Faculty of Science
University of Helsinki

CHARACTERIZATION AND SIMULATION OF MULTIPARTITE OPEN QUANTUM SYSTEMS

Marco Cattaneo

DOCTORAL DISSERTATION

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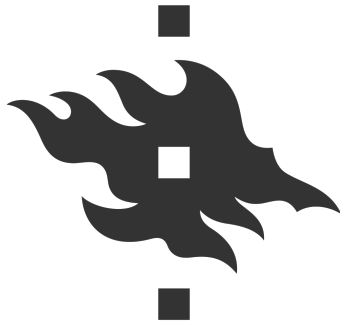
HELSINGIN YLIOPISTO

Universitat
de les Illes Balears

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OPEN QUANTUM SYSTEMS**

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DOCTORAL THESIS
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Doctoral programme in
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Characterization and simulation of multipartite open quantum systems

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Acknowledgements

At the end of all the talks I have given during my Ph.D. years, I usually put a slide with the following drawing:

$$\frac{1}{\sqrt{2}}\left(\left| \text{🏖️} \right\rangle + \left| \text{🛖} \right\rangle \right)$$

This has been my quite odd superposition state during the past four years, suspended between Palma de Mallorca and Helsinki[1]. These years have now come to an end, and my state has momentarily collapsed in the coldest branch. It is therefore also time to thank the people who made this journey possible.

First, I would like to thank my main supervisors, Roberta and Sabrina. It goes without saying that without their interest and motivation my Ph.D. would never have even started. I will always be grateful for the scientific freedom they granted me, despite the limitations of the funded research projects they are responsible for, and for their encouragement during these years. I would also like to thank my co-supervisors, Gian Luca and Matteo. They helped me many times not only with scientific problems, and they directed me towards the right numerical or analytical solution in quite a lot of situations. I believe that, if something good has appeared in our research papers during these years, it is also because my four supervisors have been extremely helpful at the right moments, perhaps each one in a different way; these disparate ways have interfered constructively for my research and, importantly, also for my personal life abroad.

I would like to thank my scientific collaborators during these years for many nice discussions and/or common works. In particular, let me thank Sorin Paraoanu, Gabriele De Chiara, Gonzalo Manzano, Jukka Pekola, Bayan Karimi, Guillermo García Pérez and Anton Trusheckhin. Thanks also to the

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[1]Although I must say, fighting stereotypes, that in Palma there are not only palms and beaches, and in Helsinki there are not only forests and snow.

members of my thesis committee at the University of Helsinki, Prof. Matteo G. A. Paris and Prof. Daniel Braun. Moreover, let me thank the pre-examiners of this thesis for their great work, who were anonymous at the University of the Balearic Islands, while they were Prof. Andrea Smirne and Dr. Javier Cerrillo at the University of Helsinki.

I would also like to thank my Ph.D. fellows, both in Spain and in Finland. The cheerful memories of the time spent in Palma with the María de Maeztu students come to my mind, as well as with the other researchers of Roberta's group and S07 room. A special mention goes to my former flatmates Jaime and Thomas, and to our intellectual cineforum (por supuesto hay que dar las gracias también a Jean-Luc Godard y al creador de Mao-Mao). In Helsinki, I was lucky enough to share my office with Nicola and Francesca[2]. I will always thank Francesca for backing me against Nicola when he is saying something crazy, and Nicola for backing me against Francesca when she is doing the same.

Thanks for their multi-colored support to my friends in Italy, and to the ones who are currently living in some hostile European countries that I will not mention due to political correctness.

Vorrei ringraziare la mia famiglia per tutto il sostegno che mi ha dato in questi anni (commenti ironici sul mio stato lavorativo inclusi!) e in quelli precedenti. Grazie ai miei genitori anche per come mi accolgono quando torno a casa, nonostante ciò mi faccia ingrassare almeno due volte all'anno.

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[2]It has been a good excuse to avoid learning Finnish, at least so far, and a good way not to lose my Italian.

Contents

Abstract

Having a quick look at contemporary quantum mechanics, we immediately see that the study of open quantum systems is of great relevance both for fundamental reasons and for the development of quantum technologies that will be able to display quantum advantage. An open quantum system is defined in a very general way as a non-isolated quantum system that is interacting with one or more external environments. This picture can give us a valuable insight, for instance, into how a single superconducting qubit of a quantum computer that is subject to thermal fluctuations loses its coherences, or into the thermodynamics of an atom immersed in the electromagnetic field. Hence, improving our understanding of the dynamics and characterization of open quantum systems is a crucial challenge in the second quantum revolution, as well as a fascinating step forward in the study of the deepest concepts in Physics, such as the quantum to classical transition.

Motivated by renewed studies on dissipative collective effects, by new discoveries about the features of noise in quantum computers, and by recent experiments focused on many-qubit systems, the interest in multipartite open quantum systems has recently risen. A dissipative collective effect may be defined as the coherent interference of the emissions (and/or absorptions) of many quantum particles interacting with external environments. Multipartite open quantum systems are open systems made of multiple subsystems, which can interact with each other and at the same time may be coupled to local and/or collective environments. This type of open quantum systems plays a crucial role, for instance, in the study of "crosstalk errors" in quantum information processors, in the thermodynamic analysis of spin or harmonic oscillator chains, as well as in the description of collective phenomena such as superradiance and quantum synchronization. The characterization and simulation of the dynamics of multipartite open quantum systems is the topic of this doctoral dissertation.

This thesis consists of six original research articles and an introduction to their methodology, scope, and significance. The first two publications explore the validity and features of the so-called global and local master equations (i.e., the equations of motion for open quantum systems), which are widely

employed in quantum thermodynamics. In particular, these papers are focused on a particular type of master equation based on the "partial secular approximation", which is shown to be accurate in all regimes of validity of the standard Markovian master equation. Moreover, the symmetry properties of these master equations are discussed. The third scientific article shows how the most common examples of multipartite open quantum systems can be simulated through a platform of superconducting qubits coupled to a resistor emitting thermal noise. The fourth publication studies how different collective effects, such as quantum synchronization, subradiance and entanglement generation, can emerge in a model of two detuned qubits coupled to a common bath. The fifth research paper introduces a quantum algorithm based on a collision model that is able to simulate the most general Markovian multipartite quantum dynamics, and proves that this algorithm can be efficiently simulated on a quantum computer. Finally, the sixth publication presents the experimental implementation of this algorithm on a near-term quantum computer, and assesses both theoretically and experimentally the features of noise on the algorithm.

In conclusion, this thesis brings some relevant contributions to the field of multipartite open quantum systems, not only regarding methodological questions, but also phenomenological predictions and experimental implementations on a quantum computer. These contributions include the description and characterization of a general master equation for Markovian multipartite open quantum systems, and some new procedures for the analog and digital quantum simulation thereof.

Resumen

Echando un vistazo rápido a la mecánica cuántica contemporánea, vemos de inmediato que el estudio de los sistemas cuánticos abiertos es de gran relevancia tanto por razones fundamentales como para el desarrollo de tecnologías cuánticas que podrán mostrar "ventaja cuántica". Un sistema cuántico abierto se define de manera muy general como un sistema cuántico no aislado que interactúa con uno o más entornos. Este concepto puede llevarnos a comprender, por ejemplo, cómo un solo qubit superconductor de una computadora cuántica que está sujeta a fluctuaciones térmicas pierde sus coherencias, o la termodinámica de un átomo inmerso en el campo electromagnético. Por lo tanto, mejorar nuestra comprensión de la dinámica y caracterización de los sistemas cuánticos abiertos es un desafío crucial en la segunda revolución cuántica, así como un fascinante paso adelante en el estudio de los conceptos más profundos de la Física, como la transición del mundo cuántico al clásico.

Motivado por nuevos estudios sobre los efectos colectivos disipativos, por nuevos descubrimientos sobre las características del ruido en computadoras cuánticas y por experimentos recientes centrados en sistemas de muchos qubits, el interés en los sistemas cuánticos abiertos y multipartitos ha crecido recientemente. Un efecto colectivo disipativo puede definirse como la interferencia coherente de las emisiones (y/o absorciones) de muchas partículas cuánticas que interactúan con entornos externos. Los sistemas cuánticos abiertos y multipartitos son sistemas abiertos formados por múltiples subsistemas, que pueden interactuar entre sí y al mismo tiempo pueden acoplarse a entornos locales y/o colectivos. Este tipo de sistemas cuánticos abiertos juega un papel crucial, por ejemplo, en el estudio de "errores de crosstalk" en los procesadores de información cuántica, en el análisis termodinámico de cadenas de espín o osciladores armónicos, así como en la descripción de fenómenos colectivos como la superradiancia y la sincronización cuántica. La caracterización y simulación de la dinámica de sistemas cuánticos abiertos y multipartitos es el tema de esta tesis doctoral.

Esta tesis consta de seis artículos de investigación originales y una introducción a su metodología, alcance y significado. Las dos primeras publicaciones exploran la validez y las características de las ecuaciones maestras globales y lo-

cales (es decir, las ecuaciones de movimiento para sistemas cuánticos abiertos), que son ampliamente empleadas en la termodinámica cuántica. En particular, estos artículos se centran en un tipo particular de ecuación maestra basada en la "aproximación secular parcial", que se puede demonstrar ser precisa en todos los regímenes de validez de la ecuación maestra markoviana estándar. Además, se discuten las propiedades de simetría de estas ecuaciones maestras. El tercer artículo científico muestra cómo se pueden simular los ejemplos más comunes de sistemas cuánticos abiertos y multipartitos a través de una plataforma de qubits superconductores acoplados a una resistencia que emite ruido térmico. La cuarta publicación estudia cómo pueden surgir diferentes efectos colectivos, como la sincronización cuántica, la subradiancia y la generación de entrelazamiento cuántico, en un modelo de dos qubits desafinados acoplados a un baño común. El quinto trabajo de investigación presenta un algoritmo cuántico basado en un modelo de colisiones que es capaz de simular la dinámica cuántica multipartita y markoviana más general y demuestra que este algoritmo se puede simular de manera eficiente en una computadora cuántica. Finalmente, la sexta publicación presenta la implementación experimental de este algoritmo en una computadora cuántica "near-term" y evalúa de manera tanto teórica como experimental las características del ruido en este algoritmo.

En conclusión, esta tesis presenta algunas contribuciones relevantes en el campo de los sistemas cuánticos abiertos y multipartitos, no solo con respecto a las cuestiones metodológicas, sino también a las predicciones fenomenológicas y a las implementaciones experimentales en una computadora cuántica. Estas contribuciones incluyen la descripción y caracterización de una ecuación maestra general para sistemas cuánticos abiertos y multipartitos markovianos, y algunos nuevos procedimientos para la simulación cuántica analógica y digital de los mismos.

Resum

Donant un cop d'ull a la mecànica quàntica contemporània, immediatament reconeixem que l'estudi dels sistemes quàntics oberts és de gran rellevància tant per raons fonamentals com per al desenvolupament de tecnologies quàntiques que podran mostrar avantatges quàntiques. Un sistema quàntic obert es defineix d'una manera molt general com un sistema quàntic no aïllat que està interactuant amb un o més entorns externs. Aquesta imatge ens pot donar una visió valuosa, per exemple, de com un únic qubit superconductor d'un ordinador quàntic que està subjecte a fluctuacions tèrmiques perd les seves coherències, o de la termodinàmica d'un àtom immers en el camp electromagnètic. Per tant, millorar la nostra comprensió de la dinàmica i la caracterització dels sistemes quàntics oberts és un repte crucial en la segona revolució quàntica, així com un pas endavant fascinant en l'estudi dels conceptes més profunds de la Física, com ara la transició de la física quàntica a clàssica.

Motivat per nous estudis sobre efectes col·lectius dissipatius, per nous descobriments sobre les característiques del soroll en ordinadors quàntics i per experiments recents centrats en sistemes de molts qubits, l'interès pels sistemes quàntics oberts multipartits ha augmentat recentment. Un efecte col·lectiu dissipatiu es pot definir com la interferència coherent de les emissions (i/o absorcions) de moltes partícules quàntiques que interactuen amb entorns externs. Els sistemes quàntics oberts multipartits són sistemes oberts formats per múltiples subsistemes, que poden interactuar entre ells i al mateix temps es poden acoblar a entorns locals i/o col·lectius. Aquest tipus de sistemes quàntics oberts tenen un paper crucial, per exemple, en l'estudi dels "errors per acoblaments" en els processadors d'informació quàntica, en l'anàlisi termodinàmica de cadenes d'oscil·ladors harmònics o de spin, així com en la descripció de fenòmens col·lectius com la superradiància, i la sincronització quàntica. La caracterització i simulació de la dinàmica de sistemes quàntics oberts multipartits és el tema d'aquesta tesi doctoral.

Aquesta tesi consta de sis articles de recerca originals i una introducció a la seva metodologia, abast i importància. Les dues primeres publicacions exploren la validesa i les característiques de les anomenades equacions mestres

globals i locals (és a dir, les equacions de moviment per a sistemes quàntics oberts), que són àmpliament emprades en termodinàmica quàntica. En particular, aquests articles es centren en un tipus particular d'equació mestra basada en l'"aproximació secular parcial", que es demostra que és precisa en tots els règims de validesa de l'equació mestra de Markoviana estàndard. A més, es discuteixen les propietats de simetria d'aquestes equacions mestres. El tercer article científic mostra com es poden simular els exemples més comuns de sistemes quàntics oberts multipartits mitjançant una plataforma de qubits superconductors acoblats a una resistència que emet soroll tèrmic. La quarta publicació estudia com diferents efectes col·lectius, com ara la sincronització quàntica, la subradiància i la generació d'entrellaçament, poden sorgir en un model de dos qubits desajustats acoblats a un bany comú. El cinquè treball de recerca introdueix un algorisme quàntic basat en un model de col·lisió que és capaç de simular la dinàmica quàntica multipartita de Markoviana més general, i demostra que aquest algorisme es pot simular de manera eficient en un ordinador quàntic. Finalment, la sisena publicació presenta la implementació experimental d'aquest algorisme en un ordinador quàntic a curt termini, i avalua tant teòricament com experimentalment les característiques del soroll a l'algorisme.

En conclusió, aquesta tesi aporta algunes contribucions rellevants al camp dels sistemes quàntics oberts multipartits, tant en qüestions metodològiques, prediccions fenomenològiques com també una implementació experimental en un ordinador quàntic. Aquestes contribucions inclouen la descripció i caracterització d'una equació mestra general per a sistemes quàntics oberts multipartits de Markov, i alguns nous procediments per a la seva simulació quàntica analògica i digital.

Tiivistelmä

Kun tarkastellaan nopeasti nykyaikaista kvanttimekaniikkaa, huomaamme heti, että avoimien kvanttijärjestelmien tutkiminen on erittäin tärkeää sekä perustavanlaatuisista syistä että kvanttietujen näyttämisen mahdollistavien kvanttiteknologioiden kehittämisen kannalta. Avoin kvanttijärjestelmä määritellään yleisellä tavalla eristämättömäksi kvanttijärjestelmäksi, joka on vuorovaikutuksessa yhden tai useamman ulkoisen ympäristön kanssa. Tämä kuva voi antaa meille arvokkaan käsityksen esimerkiksi siitä, kuinka lämpövaihteluille riippuvainen suprajohtava kubitti kvanttitietokoneessa menettää koherenssinsa tai sähkömagneettiseen kenttään upotetun atomin termodynamiikasta. Näin ollen ymmärryksemme parantaminen avoimien kvanttijärjestelmien dynamiikan ja karakterisoinnin suhteen on ratkaiseva haaste toisessa kvanttivallankumouksessa sekä kiehtova edistysaskel fysiikan syvimpien käsitteiden, kuten kvanttimekaniikan ja klassisen mekaniikan rajan, tutkimisessa.

Uusiutuneiden dissipatiivisten kollektiivisten vuorovaikutusten tutkimusten, kvanttitietokoneiden kohinan ominaisuuksista tehtyjen uusien löytöjen ja viimeaikaisten monikubittisiin järjestelmiin keskittyneiden kokeiden seurauksena kiinnostus moniosaisiin avoimiin kvanttijärjestelmiin kohtaan on viime aikoina lisääntynyt. Dissipatiivinen kollektiivinen vuorovaikutus voidaan määritellä monien ulkoisen ympäristön kanssa vuorovaikutuksessa olevien kvanttihiukkasten emission (ja/tai absorption) koherentiksi häiriöksi. Moniosaiset avoimet kvanttijärjestelmät ovat avoimia järjestelmiä, jotka koostuvat useista osajärjestelmistä, jotka voivat olla vuorovaikutuksessa toistensa kanssa ja samalla kytkeytyä paikallisiin ja/tai kollektiivisiin ympäristöihin. Tämän tyyppisillä avoimilla kvanttijärjestelmillä on ratkaiseva rooli esimerkiksi kvanttitietojen prosessorien "ylikuulumisvirheiden" tutkimuksessa, spin- tai harmonisten oskillaattoriketjujen termodynaamisessa analyysissä sekä kollektiivisten ilmiöiden, kuten supersäteilyn ja kvanttisynkronoinnin kuvauksessa. Moniosaisten avoimien kvanttijärjestelmien dynamiikan karakterisointi ja simulointi on tämän väitöskirjan aiheena.

Tämä opinnäytetyö koostuu kuudesta alkuperäisestä tutkimusartikkelista ja johdannosta niiden metodologiaan, laajuuteen ja merkitykseen. Kaksi ensimmäistä julkaisua tutkivat niin kutsuttujen globaalien ja paikallisten

pääyhtälöiden (eli avoimien kvanttijärjestelmien liikeyhtälöiden) pätevyyttä ja ominaisuuksia, joita käytetään laajalti kvanttitermodynamiikassa. Erityisesti nämä artikkelit keskittyvät tietyntyyppiseen pääyhtälöön, joka perustuu osittaiseen maalliseen approksimaatioon, joka on osoitettu olevan tarkka kaikissa standardin Markovin pääyhtälön kelpoisuusjärjestelmissä. Lisäksi käsitellään näiden pääyhtälöiden symmetriaominaisuuksia. Kolmas tieteellinen artikkeli osoittaa, kuinka yleisimpiä esimerkkejä moniosaisista avoimista kvanttijärjestelmistä voidaan simuloida suprajohtavien kubittien alustalla, joka on kytketty lämpökohinaa lähettävään vastukseen. Neljännessä julkaisussa tutkitaan, kuinka erilaiset kollektiiviset efektit, kuten kvanttisynkronointi, subradianssi ja takertuminen, voivat syntyä mallissa, jossa kaksi viritettyä kubittia on kytketty yhteiseen kylpyyn. Viides tutkimusartikkeli esittelee törmäysmalliin perustuvan kvanttialgoritmin, joka pystyy simuloimaan yleisintä Markovin moniosaista kvanttidynamiikkaa ja todistaa, että tämä algoritmi voidaan simuloida tehokkaasti kvanttitietokoneella.

Lopuksi, kuudes julkaisu esittelee tämän algoritmin kokeellisen toteutuksen lähiajan kvanttitietokoneella ja arvioi sekä teoreettisesti että kokeellisesti algoritmin kohinan ominaisuuksia. Yhteenvetona voidaan todeta, että tämä opinnäytetyö tuo olennaisia panoksia moniosaisten avoimien kvanttijärjestelmien alaan ei pelkästään metodologisessa mielessä, mutta myös fenomenologisia ennusteita kokeellisille toteutuksille kvanttitietokoneella. Nämä panokset sisältävät yleisen pääyhtälön kuvauksen ja karakterisoinnin Markovin moniosaisille avoimille kvanttijärjestelmille ja uusia menetelmiä niiden analogisille ja digitaalisille kvanttisimulaatioille.

List of Publications

This thesis consists of an introduction to the topic of multipartite open quantum systems and of the following original research articles [1–6]:

I **Local versus global master equation with common and separate baths: superiority of the global approach in partial secular approximation**,
M. Cattaneo, G. Giorgi, S. Maniscalco, and R. Zambrini, New J. Phys. **21**, 113045 (2019).

II **Symmetry and block structure of the Liouvillian superoperator in partial secular approximation**,
M. Cattaneo, G. Giorgi, S. Maniscalco, and R. Zambrini, Phys. Rev. A **101**, 042108 (2020).

III **Engineering Dissipation with Resistive Elements in Circuit Quantum Electrodynamics**,
M. Cattaneo and G.-S. Paraoanu, Adv. Quantum Tech. **4**, 2100054 (2021).

IV **Bath-Induced Collective Phenomena on Superconducting Qubits: Synchronization, Subradiance, and Entanglement Generation**,
M. Cattaneo, G. Giorgi, S. Maniscalco, G.-S. Paraoanu, and R. Zambrini, Ann. Phys. (Berlin) **533**, 2100038 (2021).

V **Collision Models Can Efficiently Simulate Any Multipartite Markovian Quantum Dynamics**,
M. Cattaneo, G. De Chiara, S. Maniscalco, R. Zambrini, and G. Giorgi, Phys. Rev. Lett. **126**, 130403 (2021).

VI **Quantum simulation of dissipative collective effects on noisy quantum computers**,
M. Cattaneo, M. A. C. Rossi, G. García-Pérez, R. Zambrini and S. Maniscalco, preprint arXiv:2201.11597 (2022).

The doctoral candidate has contributed independently and significantly to the definition of the research goals, to the study of the literature, to the analytical and numerical computations, and to the writing of all the above-listed research articles. These research papers have not been used in previous doctoral dissertations.

Other published material

This is a list of the publications co-authored by the doctoral student during his undergraduate and postgraduate studies that have not been chosen as a part of this doctoral thesis:

- **Hybrid quantum key distribution using coherent states and photon-number-resolving detectors**,
  M. Cattaneo, M. G. A. Paris, and S. Olivares, Phys. Rev. A **98**, 012333 (2018).

- **Quantum spatial search on graphs subject to dynamical noise**,
  M. Cattaneo, M. A. C. Rossi, M. G. A. Paris, and S. Maniscalco, Phys. Rev. A **98**, 052347 (2018).

- **Non-Markovianity is not a resource for quantum spatial search on a star graph subject to generalized percolation**,
  M. A. C. Rossi, *M. Cattaneo*, M. G. A. Paris, and S. Maniscalco, Quantum Meas. Quantum Metr. **5**, 40-49 (2018).

- **Comment on "Steady-State Coherences by Composite System-Bath Interactions"**,
  M. Cattaneo and G. Manzano, preprint arXiv:2106.09138 (2021).

- **Dynamics of a dispersively coupled transmon qubit in the presence of a noise source embedded in the control line**,
  A. Vaaranta, *M. Cattaneo*, and R. Lake, Phys. Rev. A **106**, 042605 (2022).

- **A brief journey through collision models for multipartite open quantum dynamics**,
  M. Cattaneo, G. Giorgi, R. Zambrini, and S. Maniscalco, Open Syst. Inf. Dyn. **29**, 2250015 (2022).

Chapter 1

Introduction

The perfect preparation, manipulation and measurement of individual quanta are the Holy Grail of the second quantum revolution, which would lead to a scalable fault-tolerant quantum computer and to quantum advantage on a plethora of tasks, including the simulation of the dynamics of many-body quantum systems. However, since the very early days of quantum information and computing scientists discovered that it is impossible to isolate a single quantum system from its surroundings. The quantum particle we aim to manipulate quickly gets entangled with many other quantum systems with which it inevitably interacts, leading to a phenomenon known as *decoherence* [7]. This jeopardizes the local "quantumness" of the quantum particles, and therefore hinders the quantum operations we need to perform in order to achieve advantage with respect to applications based on systems operating in the classical regime. These considerations boosted the study of the theory of open quantum systems [8], although the origins of this field can be traced back to the very early days of modern quantum mechanics [9].

An open quantum system interacts with some (or many) quantum particles around it, which are usually referred to as "the environment". For this reason, the dynamics of the state of the system alone is not characterized by the standard Schrödinger equation anymore, but it needs a more sophisticated description. A typical example of an open quantum system is a single trapped ion or an individual superconducting qubit interacting with the external electromagnetic field.

The theory of open quantum systems is nowadays a well-consolidated framework whose fruitful results have been collected in different books on the topic [8, 10–14]. The Markovian and non-Markovian dynamics of, for instance, a single spin or a bosonic field immersed in a thermal or squeezed bath is well understood [8]. A less studied problem is the evolution of a *multipartite* open quantum system. That is, a structured open quantum system composed

of multiple subsystems that interact with local and/or collective baths. The characterization and quantum simulation of this kind of open quantum systems is the subject of this doctoral thesis.

The interest in multipartite open quantum systems has grown in recent years due to a number of reasons. For instance, "cross-talk errors" have been found to play a relevant role in the noise of quantum computers [15–17]. These are non-local errors that affect more than one qubit at a time and may be due to the operations performed on distant qubits. To properly characterize the noise that generates cross-talk errors, we inevitably have to describe the qubits of the quantum computer as a multipartite open quantum system interacting with a highly non-local bath.

The characterization of the environment as an enemy for quantum computation is not the only motivation for the study of multipartite open quantum systems. Indeed, already twenty years ago it was shown that the environment can also act as a friend: if engineered in a proper way, a collective environment on multiple subsystems can generate decoherence-free-subspaces [18, 19], i.e., subspaces of the Hilbert space of the multipartite open quantum system where the dynamics is fully unitary, and dissipation and decoherence do not emerge.

Multipartite open quantum systems are also of great interest for the growing study of dissipative collective phenomena, such as superradiance [20–22] or subradiance [23] in a structured atomic system, the dissipation-driven synchronization of quantum particles [24], or dissipative quantum phase transitions [25]. Last but not least, the study of multipartite open quantum systems is particularly relevant for quantum thermodynamics. Understanding how heat, work and entropy are exchanged in structured open systems, and how the latter reach thermalization depending on their internal interaction and on the non-locality of the thermal baths they are immersed in, is not a trivial task. For instance, an important discussion has arisen few years ago (and it is still partially ongoing) on which master equations are suitable for the description of multipartite open quantum systems, and, specifically, on which of them fulfill the laws of quantum thermodynamics [26–30].

Building a complete and comprehensive theory of multipartite open quantum systems is a formidable task that will require a collective effort of the scientific community for some decades. This thesis is intended to provide a solid contribution to this effort. More specifically, the research questions we will address are the following:

1. What is a sufficiently general class of Markovian master equations for the accurate description of multipartite open quantum systems? What are their properties? What are their symmetries, if any? What are the physical systems to which they apply?

2. Are there some interesting collective effects that are captured by this

class of master equations?

3. How can we simulate some examples of multipartite open quantum systems using a superconducting qubit platform?

4. Can we find a general algorithm to simulate multipartite open quantum systems on a quantum computer?

5. How is the performance of such an algorithm on the currently available near-term quantum computers? What are the noise limitations thereof?

Publication **I** and Publication **II** address the first research question. In particular, they discuss the validity of a Markovian master equation derived under the so-called *partial secular approximation*, and they explore its physical and mathematical properties. Publication **III** deals with the third research question and, inspired by the experimental works of collaborators at Aalto University, shows how resistive elements in superconducting circuits can be employed to engineer an analog simulation of multipartite open quantum systems immersed in thermal baths. Publication **IV** builds on the results of Publications **I**, **II** and **III** and, addressing the second research question, shows how subradiance, quantum synchronization and environment-mediated entanglement generation can be observed on a pair of superconducting transmon qubits coupled to a common resistor. Publication **V** provides a complete and satisfactory answer to the fourth research question by putting forward an algorithm based on a so-called *collision model* that is able to simulate the most general Markovian dynamics of a multipartite open quantum system. The relevance of the *multipartite collision model* is not restricted to quantum simulation, as this protocol may be of interest also for the kinetic description of the thermalization of a multipartite open quantum system and for the study of its quantum thermodynamic properties. Finally, the experimental results on a near-term quantum computer presented in Publication **VI** answer the fifth research question. Moreover, Publication **VI** provides a both theoretical and experimental noise analysis for the errors of the multipartite collision model.

The structure of this doctoral dissertation is the following. In Chapter 2 we briefly introduce the most relevant theoretical tools to study multipartite open quantum systems, so as to provide the reader with the necessary notions to go through the results of this thesis. The scope and the findings of the research papers that are part of this dissertation are discussed in Chapter 3 without getting into the details, roughly following the research questions that we have listed above. Chapter 3 also quickly discusses the background of these research questions and the most recent developments in the field. Some concluding remarks are drawn in Chapter 4. Finally, the original publications that are part of this doctoral thesis are attached at the end of this manuscript,

and the reader can find there the details and the derivations of all the results of this dissertation.

Chapter 2

Theoretical methods

In this chapter, we introduce the main theoretical tools that we need to study the characterization and simulation of multipartite open quantum systems. First, we will quickly present the concept of quantum dynamical maps[1], which is at the basis of the theory of quantum information and quantum computation. We will then discuss how we can introduce different figures of merit to determine how different two quantum maps are. After that, we will present the general structure of a Markovian master equation for the dynamics of an open quantum system. We will also focus on how the ideas of "symmetry" and "conserved quantity" can be introduced in the evolution generated by this master equation. After reviewing the formalism of open system quantum mechanics in the Liouville space, we will see how a Markovian master equation can be derived starting from the microscopic model of an open quantum system weakly coupled to an external environment. Finally, we will observe that the same kind of master equation can be simulated through a very particular type of quantum maps, namely the *collision models*.

2.1 Quantum states and quantum dynamical maps

Following textbook quantum mechanics [31, 32], we postulate that the state of a quantum system is completely described by its *density matrix* ρ, which lives in the convex set $\mathcal{S}(\mathcal{H})$ characterized as:

$$\mathcal{S}(\mathcal{H}) = \{\rho \in \mathcal{B}(\mathcal{H}) \text{ such that } \rho \geq 0, \ \mathrm{Tr}[\rho] = 1\}, \tag{2.1}$$

---

[1]Equivalently, we will also employ the terms "quantum operation" and "quantum channel". Although their definitions may vary depending on the textbook and scientific community, in this thesis we will make use of these terms and of "quantum map" as if they were synonyms. In particular, for simplicity we will assume they all refer to trace-preserving maps.

where $\mathcal{B}(\mathcal{H})$ is the space of bounded operators on the Hilbert space of the system $\mathcal{H}$. For simplicity, the investigation throughout the thesis will involve only finite-dimensional system Hilbert spaces $\mathcal{H}$, therefore ρ has always a well-defined trace. Since ρ is a semi-positive operator, it can always be diagonalized and written as

$$\rho = \sum_{j=1}^{d} c_j \, |v_j\rangle\langle v_j| , \tag{2.2}$$

where $d = \dim(\mathcal{H})$ and $c_j \geq 0$, $\sum_{j=1}^{d} c_j = 1$. Eq. (2.2) provides us with a convenient interpretation of the density matrix: the most general description of a quantum system can be thought of as a convex "incoherent" combination of a set of physical states $|v_j\rangle \in \mathcal{H}$, each of them picked with a probability c_j. In this way, we are putting forward a fully probabilistic interpretation of the density matrix as a mathematical object to describe our classical uncertainty (i.e., the probabilities $\{c_j\}_{j=1}^{d}$) on the "real" physical state of the system, which is characterized by a vector in $\mathcal{H}$.

After introducing the general description of the state of a quantum system, we run into another crucial postulate of quantum mechanics. The evolution of the density matrix ρ in time for a closed quantum system, $\rho(t)$, is driven by the von Neumann equation, at least if no measurements are performed on the quantum system [31]:

$$\frac{d}{dt}\rho(t) = -\frac{i}{\hbar}[H, \rho(t)], \tag{2.3}$$

where H is the system Hamiltonian, which, for simplicity, is time-independent. The dynamics of $\rho(t)$ can also be expressed as:

$$\rho(t) = \mathcal{U}(t)[\rho(0)] = U(t)\rho(0)U^{\dagger}(t), \tag{2.4}$$

where $U(t)$ is a unitary operator derived from Eq. (2.3), which can be written as:

$$U(t) = e^{-\frac{i}{\hbar}Ht}. \tag{2.5}$$

$\mathcal{U}(t)$ is a linear operator acting on $\mathcal{B}(\mathcal{H})$, therefore we will refer to it as a *superoperator*.

Let us now consider the quantum state of a subsystem of $\mathcal{H}$ only. This is obtained through a mathematical operation called *partial trace* [7, 8], which can be thought of as the generalization of the marginal probability distribution in classical statistical mechanics to quantum physics:

$$\rho_S(t) = \mathrm{Tr}_E[\rho(t)], \tag{2.6}$$

where we label as "S" the subsystem we are interested in, and as "E" all the complementary subsystems in $\mathcal{H}$, such that we can decompose the latter as

$\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E$. This conceptual separation of the Hilbert space of the overall quantum system $\mathcal{H}$ is at the basis of the theory of open quantum systems [8]. Indeed, from now we will refer to S as the "(open) system" and to E as the "environment" into which S is immersed. Typically, we are interested in the dynamics and characterization of S only, while we do not aim to monitor the state of the environment at each instant of time.

A key issue of the theory of open quantum systems is the fact that we cannot write an evolution driven by the von Neumann master equation as in Eq. (2.4) for the reduced state $\rho_S(t)$. A quick look at Eq. (2.6), indeed, reveals that the evolution of $\rho_S(t)$ is in general non-unitary. We therefore have to introduce a more general set of operations beyond the unitary superoperator $\mathcal{U}(t)$ to be able to describe the evolution of an open quantum system. We will refer to this as the set of *quantum maps*[2] $\phi : \mathcal{B}(\mathcal{H}_S) \to \mathcal{B}(\mathcal{H}_S)$, defined by the following three properties:

Linearity Recalling the interpretation of a density matrix as a classical average of pure quantum states in Eq. (2.2), making the overall density matrix ρ_S evolve must correspond to implementing the evolution of each pure state $|v_j\rangle$ in the convex combination ρ_S and then taking the classical average of the evolved states. That is, the map must be linear:

$$\phi[A + B] = \phi[A] + \phi[B] \ \text{ for all } A, B \in \mathcal{B}(\mathcal{H}_S). \tag{2.7}$$

Trace-Preserving When we apply the evolution ϕ on a physical quantum state, we expect to obtain another physical quantum state. Density matrices associated with physical states have trace equal to 1, therefore we assume:

$$\mathrm{Tr}[\phi[A]] = \mathrm{Tr}[A] \ \text{ for all } A \in \mathcal{B}(\mathcal{H}_S). \tag{2.8}$$

Complete positivity Following the same reasoning as for the trace-preserving property, the output of a quantum map applied to a physical state must be a semipositive-definite density matrix (i.e., the map must be positive). Moreover, the same must hold when we consider the quantum map $\phi \otimes \mathbb{I}_C$ on a general dilation of the Hilbert space of the system only. Indeed, a local evolution of an entangled state living in both S and the dilated space C must still yield a physical density matrix. This is captured by a property called *complete positivity*:

$$\phi \otimes \mathbb{I}_{\mathbb{C}^{k \times k}} \geq 0 \ \text{ for all } k \geq 0. \tag{2.9}$$

---

[2] Note that, for simplicity, we are defining both the domain and codomain of ϕ as the space of bounded operators on $\mathcal{H}_S$. We will see that this will be particularly convenient when solving the dynamics of an open quantum system. However, physically we should always think of ϕ as being applied to density matrices in $\mathcal{S}(\mathcal{H}_S)$ and returning density matrices.

Because of these properties, the quantum maps are also often called "completely positive trace preserving (CPTP) maps".

The "physical version" [7, 33] of a well-known theorem by Stinespring [34] on completely positive maps states that every quantum map can be written as:

$$\phi[\rho_S] = \mathrm{Tr}_E[U_I \rho_S \otimes \rho_E U_I^\dagger], \tag{2.10}$$

where $\mathcal{H}_E$ is a Hilbert space, ρ_E is a density matrix in $\mathcal{S}(\mathcal{H}_E)$ and U_I is a suitable unitary operator acting on the *dilated* Hilbert space $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E$. By making U_I depend on time t, we can therefore think of any quantum map $\phi(t)$ describing the evolution of the state of the system at time t as coming from a suitable unitary dynamics between the state of the system and the state of some external environment as in Eq. (2.6), and viceversa.

Finally, we provide yet another useful characterization of a quantum map ϕ by introducing the *Choi matrix* Φ [35]. It can be shown that there is an isomorphism between any CPTP quantum map ϕ acting on the operators on a d_S-dimensional Hilbert space $\mathcal{H}_S$ and a positive definite $d_S^2 \times d_S^2$ matrix Φ defined by:

$$\Phi = \begin{pmatrix} \phi(|e_1\rangle\langle e_1|) & \dots & \phi(|e_1\rangle\langle e_{d_S}|) \\ \vdots & \ddots & \vdots \\ \phi(|e_{d_S}\rangle\langle e_1|) & \dots & \phi(|e_{d_S}\rangle\langle e_{d_S}|) \end{pmatrix}, \tag{2.11}$$

where $\{|e_j\rangle\}_{j=1}^{d_S}$ is the canonical basis of $\mathcal{H}_S$, i.e., $|e_1\rangle = (1, 0, \dots, 0)^T$, and so on. Analogously, we can write the Choi matrix as $\Phi = \sum_{j,k=1}^{d_S} |e_j\rangle\langle e_k| \otimes \phi(|e_j\rangle\langle e_k|)$.

2.2 Distances between quantum maps

As discussed in the previous section, the most general dynamics of an open quantum system initialized in a state not correlated with the environment is driven by a CPTP quantum map ϕ. In particular, we may think of implementing a certain quantum simulation algorithm on a quantum computer, and the ideal evolution until time t simulated by this quantum algorithm may be represented as a quantum map $\phi(t)$. When the algorithm will be implemented on a real quantum computer, however, we will most likely find out that noise and errors in the device will have affected the accuracy of the quantum simulation algorithm. As a consequence, the actual evolution until time t will not be described anymore by the ideal $\phi(t)$, but by a different quantum map $\phi^*(t)$ that characterizes the noisy dynamics. The mismatch between $\phi(t)$ and $\phi^*(t)$ can be thought of as the error of the quantum simulation algorithm due to the noise on the quantum computer we are using in the laboratory. Hence,

we are interested in introducing some measures of "how distant" two quantum channels are. This is what we will briefly study in this section.

First of all, let us quickly define which are the most employed measures of distance between two quantum states. To do this, we need to introduce the so-called Schatten norms for operators in $\mathcal{B}(\mathcal{H}_S)$ [36, 37].

Definition 1 (Schatten norms). The Schatten p-norm (where $p \in [1, \infty]$) of $A \in \mathcal{B}(\mathcal{H}_S)$ is given by:

$$\|A\|_p = \text{Tr}\left[\left(\sqrt{A^\dagger A}\right)^p\right]^{\frac{1}{p}}. \tag{2.12}$$

For our purposes, it is sufficient to focus on the cases $p = 1$ and $p = \infty$:

Definition 2 (Trace norm). The trace norm of an operator $A \in \mathcal{B}(\mathcal{H}_S)$ is the Schatten 1-norm:

$$\|A\|_1 = \text{Tr}\left[\sqrt{A^\dagger A}\right]. \tag{2.13}$$

Definition 3 (Operator norm). The operator norm (or infinity norm) of $A \in \mathcal{B}(\mathcal{H}_S)$ is the Schatten ∞-norm:

$$\|A\|_\infty = \max_{|v\rangle \in \mathcal{H}_S : \|v\| = 1} \|A |v\rangle\|. \tag{2.14}$$

The vector norm (without any subscript) $\|v\|$ is the standard Euclidean norm in the Hilbert space $\mathcal{H}_S$.

Two key properties of these Schatten norms will be particularly useful for our discussion [38]:

$$\begin{aligned} \|A \otimes \mathbb{I}_B\|_\infty &= \|A\|_\infty, \quad \|A \otimes \mathbb{I}_B\|_1 = d_B \|A\|_1, \\ \|\text{Tr}_B[X_{SB}]\|_\infty &\leq d_B \|X_{SB}\|_\infty, \quad \|\text{Tr}_B[X_{SB}]\|_1 \leq \|X_{SB}\|_1, \end{aligned} \tag{2.15}$$

for all $A \in \mathcal{B}(\mathcal{H}_S)$ and all $X_{SB} \in \mathcal{B}(\mathcal{H}_S \otimes \mathcal{H}_B)$, where we have introduced an additional Hilbert space $\mathcal{H}_B$ whose dimension is d_B.

By making use of the trace norm, we can introduce one of the most common measures of distance between quantum states, namely the *trace distance*:

$$T(\rho, \sigma) = \frac{1}{2} \|\rho - \sigma\|_1, \text{ with } \rho, \sigma \in \mathcal{S}(\mathcal{H}_S). \tag{2.16}$$

The trace distance is a well-defined metric on $\mathcal{S}(\mathcal{H}_S)$, it satisfies the inequality $0 \leq T(\rho, \sigma) \leq 1$, and it is equal to 1 if and only if ρ and σ are orthogonal states. It can be employed to estimate the maximum probability of distinguishing between two quantum states by making proper measurements thereon via suitable positive operator-valued measures (POVMs) [7].

Another figure of merit to estimate how different two quantum states are is the *fidelity*:

$$\mathcal{F}(\rho, \sigma) = \left\| \sqrt{\rho}\sqrt{\sigma} \right\|_1^2 = \left(\mathrm{Tr}\left[\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}} \right] \right)^2, \text{ with } \rho, \sigma \in \mathcal{S}(\mathcal{H}_S). \qquad (2.17)$$

If $\rho = |\psi\rangle\langle\psi|$ is pure, then $\mathcal{F}(\rho, \sigma) = \mathrm{Tr}[\rho\sigma]$. The fidelity of two quantum states goes from 0 to 1, and it is 1 if and only if $\rho = \sigma$. However, the *infidelity* $1 - \mathcal{F}(\rho, \sigma)$ is not a well-defined mathematical distance because it does not satisfy the triangle inequality.

The infidelity and the trace distance between two quantum states are connected through the following inequality:

$$1 - \sqrt{\mathcal{F}(\rho, \sigma)} \le T(\rho, \sigma) \le \sqrt{1 - \mathcal{F}(\rho, \sigma)}. \qquad (2.18)$$

Let us now address the distance between two quantum maps ϕ_1 and ϕ_2. A quite intuitive figure of merit is based on *one-to-one superoperator norm*:

Definition 4 (One-to-one superoperator norm)**.**

$$\|\mathcal{T}\|_{1\to1} = \max_{\|\rho\|_1=1} \|\mathcal{T}[\rho]\|_1, \qquad (2.19)$$

where $\mathcal{T}$ is a generic linear bounded superoperator (it does not have to be a quantum map). If we set $\mathcal{T} = \phi_1 - \phi_2$, then we can introduce a proper mathematical distance between these channels.

According to Eq. (2.15), the $1 \to 1$ superoperator norm of the tensor product between an operator on $\mathcal{H}_S$ and the identity on an additional Hilbert space is proportional to the dimension of the latter. This leads us to the quite counter-intuitive notion that the $1 \to 1$ distance between two quantum channels depends on whether or not there is an additional identity channel acting on an extended Hilbert space. This suggests that we should look for a more refined distance between quantum maps. We can notice that the definition in Eq. (2.19) is based on the trace distance between two quantum states, which, as previously said, is related to the capability of distinguishing between them. However, a CPTP map is still positive when an additional tensor product with the identity on a bigger Hilbert space is introduced. Therefore, we can make use of this property to distinguish between entangled quantum states living in a dilated Hilbert space. These considerations lead us to the *diamond norm* [36, 37]:

Definition 5 (Diamond norm)**.** The diamond norm of a superoperator $\mathcal{T}$ is defined as:

$$\|\mathcal{T}\|_{\diamond} = \|\mathcal{T} \otimes \mathbb{I}_A\|_{1\to1}, \qquad (2.20)$$

where $\mathbb{I}_A$ is the identity superoperator over a copy of the space $\mathcal{B}(\mathcal{H}_S)$. It can be shown that $\|\mathcal{T} \otimes \mathbb{I}_B\|_\diamond = \|\mathcal{T}\|_\diamond$ for all dilations $\mathcal{H}_B$. The diamond norm is usually computed through a semidefinite program [39].

Starting from the diamond norm, we can introduce the corresponding mathematical distance between quantum maps:

Definition 6 (Diamond distance). The diamond distance between ϕ_1 and ϕ_2 is

$$d_\diamond(\phi_1, \phi_2) = \frac{1}{2}\|\phi_1 - \phi_2\|_\diamond. \tag{2.21}$$

Another relevant figure of merit to estimate how far two quantum maps are is the *average gate fidelity*, which is very often used for characterizing quantum computers, and is defined between a unitary superoperator $\mathcal{U}_g$ (the "gate") and a generic quantum channel ϕ:

Definition 7 (Average gate fidelity). If $\mathcal{U}_g$ is the unitary superoperator associated with a quantum gate and ϕ is a noisy implementation thereof, the average gate fidelity is [40]:

$$
\begin{aligned}
\varphi(\mathcal{U}_g, \phi) &= \int d\mu(\psi)\mathcal{F}(\mathcal{U}_g[|\psi\rangle\langle\psi|], \phi[|\psi\rangle\langle\psi|]) \\
&= \int d\mu(\psi)\langle\psi|\mathcal{U}_g^{-1}\phi[|\psi\rangle\langle\psi|]|\psi\rangle,
\end{aligned}
\tag{2.22}
$$

where $d\mu(\psi)$ is the Haar measure over the pure states of the $\mathcal{H}_S$ and $\mathcal{F}$ is the fidelity in Eq. (2.17). The *average gate infidelity* is simply given by $r(\mathcal{U}_g, \phi) = 1 - \varphi(\mathcal{U}_g, \phi)$.

Note that, in general terms, to find the values of the average gate fidelity, of the diamond distance between an ideal gate and its noisy implementation, or of the one-to-one superoperator norm, we need perfect knowledge of the noisy map ϕ. This is obtained, for instance, by reconstructing the Choi matrix Φ (see Eq. (2.11)) associated with ϕ. To do this, we typically need to perform a quite complex quantum task called *full process tomography* [7, 41].

The average gate fidelity estimates the mismatch between the application of the physical realization of a quantum gate and of its ideal counterpart averaged over all the possible initial states. In contrast, if we employ the diamond distance to estimate the difference between these quantum maps we are considering the worst-case-scenario error [42], as the diamond norm makes use of the one-to-one norm, which in turn is computed through a maximization over all the possible states, as expressed in Eq. (2.19). An upper bound for the diamond distance based on the average gate infidelity has been introduced [43]:

$$d_\diamond(\mathcal{U}_g, \phi) \le d_S\sqrt{(1 + d_S^{-1})(r(\mathcal{U}_g, \phi))}, \tag{2.23}$$

where we recall that $d_S = \dim(\mathcal{H}_S)$. Note that the dependence between average gate infidelity and diamond norm involves a square root, exactly as between the state infidelity and the trace distance according to Eq. (2.18). The bound in Eq. (2.23) can be improved if more features of the noise in ϕ are known, see for instance Ref. [44].

2.3 Markovian dynamics of a quantum system

The most famous and successful result of the theory of open quantum systems is the description of any Markovian dynamics by means of a well-characterized master equation. Defining what "Markovianity" means in the context of the physical evolution of a quantum system is not a trivial task. Extensive studies on this problem can be found in the literature, e.g., see the reviews in Refs. [45–47]. For our purposes, we say that a quantum evolution characterized by a time-labeled family of quantum maps $\phi(t)$ is Markovian if the latter satisfies the following semigroup property:

$$\phi(t_1)\phi(t_2) = \phi(t_1 + t_2) \quad \forall t_1, t_2 \geq 0. \tag{2.24}$$

This kind of quantum map is usually referred to as a *quantum dynamical semigroup* [8, 10], with the additional physically motivated assumption $\phi(0) = \mathbb{I}_S$, i.e., without losing generality the dynamics starts at time $t = 0$.

Under reasonable mathematical assumptions [10], there exists a linear operator $\mathcal{L}$ that is the *generator* of the quantum dynamical semigroup $\phi(t)$ through:

$$\phi(t) = \exp(\mathcal{L}t). \tag{2.25}$$

In this thesis, we will refer to $\mathcal{L}$ as the *Liouvillian superoperator*. $\mathcal{L}$ is given by:

$$\mathcal{L} = \lim_{t \to 0^+} \frac{\phi(t) - \mathbb{I}_S}{t}. \tag{2.26}$$

If the state of the system at time t is obtained through the application of the quantum dynamical semigroup through $\rho_S(t) = \phi(t)[\rho_S(0)]$, then the master equation driving the system dynamics can be written as follows:

$$\frac{d}{dt}\rho_S(t) = \mathcal{L}[\rho_S(t)]. \tag{2.27}$$

Remarkably, the general structure of the master equation above is known for any $\mathcal{L}$ defined as in Eq. (2.26), that is, for any Markovian dynamics of an open quantum system ρ_S. It was presented in its generality by Gorini, Kossakowski and Sudarshan [48] and independently by Lindblad in 1976 [49].

For this reason, it is broadly known as the Gorini-Kossakowski-Sudarshan-Lindblad (GKLS) master equation. If the readers are interested in the history and origin of this master equation, we refer them to Ref. [50].

The non-diagonal form of the GKLS master equation for an open system living in the Hilbert space $\mathcal{H}_S$ is given by [8, 48]:

$$\mathcal{L}[\rho_S(t)] = -\frac{i}{\hbar}[H, \rho_S(t)] + \sum_{j,k=1}^{d_S{}^2-1} \gamma_{jk} \left(F_j \rho_S(t) F_k^\dagger - \frac{1}{2}\{\rho_S(t), F_k^\dagger F_j\} \right), \quad (2.28)$$

with $d_S = \dim(\mathcal{H}_S)$. $H = H^\dagger$ is a self-adjoint operator that we call *effective Hamiltonian*. $\{F_j\}_{j=1}^{d_S{}^2-1}$ with $\mathrm{Tr}\left[F_j F_k^\dagger\right] = \delta_{jk}$ are some orthonormal traceless operators that together with the identity form a basis of $\mathcal{B}(\mathcal{H}_S)$. We refer to them as the *Gorini-Kossakowski-Sudarshan (GKS) operators*. The coefficients γ_{jk} are the elements of the semipositive *Kossakowski matrix* $\gamma \geq 0$.

Being semipositive, the Kossakowski matrix can be diagonalized through a suitable unitary matrix C. Then, if we introduce a new set of operators L_k, namely the *Lindblad operators*, through $F_j = \sum_{k=1}^{d_S{}^2-1} C_{kj} L_k$, we obtain the diagonal form of the GKLS master equation [8, 49]:

$$\mathcal{L}[\rho_S(t)] = -\frac{i}{\hbar}[H, \rho_S(t)] + \sum_{k=1}^{d_S{}^2-1} \Gamma_k \left(L_k \rho_S(t) L_k^\dagger - \frac{1}{2}\{\rho_S(t), L_k^\dagger L_k\} \right), \quad (2.29)$$

where $\Gamma_k = \sum_{j,j'=1}^{d_S{}^2-1} C_{kj} \gamma_{jj'} C_{kj'}^*$ are the *decay rates* of the master equation, which are the eigenvalues of the Kossakowsky matrix, and therefore they are non-negative.

We conclude this section by discussing the *adjoint master equation*. As for the standard framework of unitary quantum mechanics [32], it may sometimes be useful to work in the Heisenberg picture, that is, studying the time evolution of the system observables instead of the system states. Indeed, what we are interested in are ultimately the mean values of some system operator (say $A \in \mathcal{B}(\mathcal{H}_S)$) at time t:

$$\mathrm{Tr}_S[A\rho_S(t)] = \mathrm{Tr}_S[A\phi(t)[\rho_S(0)]] = \mathrm{Tr}_S[(\phi^\dagger(t)[A])\rho_S(0)] = \mathrm{Tr}_S[A_H(t)\rho_S(0)], \quad (2.30)$$

where $A_H(t)$ is the Heisenberg picture operator. If $\phi(t)$ is a quantum dynamical semigroup, the GKLS adjoint master equation for the evolution of any operator $A_H(t) \in \mathcal{B}(\mathcal{H}_S)$ is [8]:

$$\begin{aligned}
\frac{d}{dt} A_H(t) = &\mathcal{L}^\dagger[A_H(t)] = \frac{i}{\hbar}[H, A_H(t)] \\
&+ \sum_{k=1}^{d_S{}^2-1} \Gamma_k \left(L_k^\dagger A_H(t) L_k - \frac{1}{2}\{A_H(t), L_k^\dagger L_k\} \right),
\end{aligned} \quad (2.31)$$

where all the operators and coefficients are the same as in Eq. (2.29). The adjoint Liouvillian superoperator is the generator of the adjoint quantum dynamical semigroup through $\phi^\dagger(t) = \exp\left(\mathcal{L}^\dagger t\right)$.

2.4 Symmetries in open quantum systems

The notion of symmetry is crucial in any field of Physics, and the theory of open quantum systems makes no exception. Let us suppose that G is a group and $U(g)$ is a unitary representation thereof acting on the Hilbert space of the system $\mathcal{H}_S$ for any $g \in G$. Let us now consider a quantum map $\phi : \mathcal{B}(\mathcal{H}_S) \to \mathcal{B}(\mathcal{H}_S)$. We say that ϕ is *covariant* under the action of the group G if [51–53]:

$$\mathcal{U}_g \phi \mathcal{U}_g^\dagger = \phi \quad \forall g \in G, \tag{2.32}$$

or equivalently $[\mathcal{U}_g, \phi] = 0$, where we have introduced the superoperator $\mathcal{U}_g[A] = U(g)AU^\dagger(g)$ for all $A \in \mathcal{B}(\mathcal{H}_S)$. Note that this definition corresponds to:

$$\phi[U(g)\rho_S U^\dagger(g)] = \mathcal{U}_g \phi \mathcal{U}_g^\dagger[U(g)\rho_S U^\dagger(g)] = U(g)\phi[\rho_S]U^\dagger(g), \tag{2.33}$$

which justifies the term "covariance" for this property.

The notion of covariance has been widely employed to study resource theories and the constraints they impose on the evolution of open quantum systems [54–58]. Moreover, it has been observed that, crucially, Noether's theorem does not hold anymore for open quantum dynamics [59]. That is, we cannot assign a conserved quantity of the evolution to each dynamical symmetry given by Eq. (2.32).

For our purposes, it is of crucial importance to focus on the notion of covariance and its relation with conserved quantities for a quantum dynamical semigroup. This problem has been extensively discussed in two seminal papers about ten years ago [60, 61]. Given $\phi(t) = e^{\mathcal{L}t}$, Eq. (2.32) for all t is transformed into:

$$\mathcal{U}_g \mathcal{L} \mathcal{U}_g^\dagger = \mathcal{L} \text{ or equivalently } [\mathcal{U}_g, \mathcal{L}] = 0 \quad \forall g \in G, \tag{2.34}$$

which is the definition of a quantum dynamical semigroup covariant under the action of the group G. Eq. (2.34) is usually referred to as a "weak symmetry" [60] or a "symmetry on the superoperator level" [2, 61].

Let us now suppose that G is an Abelian group that can be characterized as a continuous symmetry $U(g) = \exp(igJ)$, where J is some system observable and (with abuse of notation) $g \in \mathbb{R}$. Similarly, we can write the superoperator $\mathcal{U}_g = \exp(ig\mathcal{J})$ as a one-parameter group generated by $\mathcal{J} = [J, \cdot]$.

We say that J is a *conserved quantity* of the dynamics if its mean value is constant along time, which can be rewritten as $\mathcal{L}^\dagger[J] = 0$, where we have used the adjoint GKLS master equation in Eq. (2.31). A well-known result of unitary quantum mechanics is the Noether's theorem, which states that for each symmetry (i.e., $U(g)HU^\dagger(g) = H$ where H is the system Hamiltonian) we have a conserved quantity, namely $[J, H] = 0$ such that the mean value of J does not change in time. This is in general not true for an open quantum system, and specifically for the weak symmetry of a quantum dynamical semigroup in Eq. (2.34) [60, 61]. Indeed, recalling the structure of the GKLS master equation driven by $\mathcal{L}$ in Eq. (2.29), and in particular the effective Hamiltonian H and the Lindblad operators $\{L_k\}_k$, consider the following three propositions:

1. $[H, J] = [L_k, J] = 0$ for all k.

2. $\frac{d}{dt}J_H(t) = \mathcal{L}^\dagger[J_H(t)] = 0$.

3. $\mathcal{U}_g \mathcal{L} \mathcal{U}_g^\dagger = \mathcal{L}$, or equivalently $[\mathcal{L}, \mathcal{J}] = 0$.

Then, in general we can only say that 1. implies 2. and 3. (in this case we say that there is a "strong symmetry" of the dynamics [60]), but no other implications are in general true. That is, there are some open evolutions in which a conserved quantity does not generate a weak symmetry, and some in which a weak symmetry is present but there is no conserved quantity associated with it [61].

Conserved quantities are important because they give us crucial information on the structure of the space of stationary states of the dynamics [60–63]. In contrast, the symmetries or covariances of the dynamics can help us to simplify the solution of the GKLS master equation we are interested in. Indeed, the property $[\mathcal{L}, \mathcal{J}] = 0$ tells us that the Liouvillian superoperator and the superoperator $\mathcal{J}$ share a common basis of eigenvectors, and typically the eigenvalues and eigenvectors of $\mathcal{J}$ are known. We will see how to exploit this property to reduce the effective dimension of the Liouvillian superoperator in the next section.

2.5   The Liouville space formalism

The Liouvillian superoperator introduced in Eq. (2.26) is by definition a linear operator acting on the Hilbert space $\mathcal{B}(\mathcal{H}_S)$. Therefore, it is natural to represent it as a matrix acting on the vectorized elements of $\mathcal{B}(\mathcal{H}_S)$. If $\dim(\mathcal{H}_S) = d_S$, then the elements of $\mathcal{B}(\mathcal{H}_S)$ are usually represented as $d_S \times d_S$ matrices, while the Liouvillian can be represented as a $d_S{}^2 \times d_S{}^2$ matrix. Strictly speaking, the Liouville space is the vectorized space of operators on

the Hilbert space of the system $\mathcal{B}(\mathcal{H}_S)$, which now become d_S^2-dimensional vectors. Therefore, the Liouvillian superoperator is an operator acting on the Liouville space. In this section, we briefly review the formalism of open quantum systems in the Liouville space focusing on the results that are important for this thesis, and we refer the readers interested in the mathematical details to the excellent tutorial by Gyamfi [64].

A pure quantum state in $\mathcal{H}_S$ is represented by a ket $|v\rangle$ [31, 32]. In this language, the elements of $\mathcal{B}(\mathcal{H}_S)$ (including the density matrices according to Eq. (2.2)) are written as

$$O = \sum_{j,k=1}^{d_S} O_{jk} |v_j\rangle \langle v_k|, \tag{2.35}$$

where $\{|v\rangle_j\}_{j=1}^{d_S}$ is a basis of $\mathcal{H}_S$ and O_{jk} are the elements of the matrix associated with O and written in the same basis, such that $O|v_m\rangle = \sum_j O_{jm} |v_j\rangle$. Our aim is to write O as a vector. To do so, we apply the following "bra-flipping" transformation [64]:

$$O \to \|O\rangle\rangle = \sum_{j,k=1}^{d_S} O_{jk} |v_j\rangle \otimes |v_k\rangle. \tag{2.36}$$

In other words, we are introducing a tensor product notation to transform the operator O into a vector. The bras are transformed into new kets that are vectors in a copy of the Hilbert space $\mathcal{H}_S$. Since the dual space of the bras is isomorphic to $\mathcal{H}_S$, this transformation is always well-defined. Moreover, note that it is basis-independent, as it can be written through a suitable linear superoperator acting on $\mathcal{B}(\mathcal{H}_S)$ [64].

Let us now derive some useful identities in this new formalism. First of all, the Hilbert-Schmidt inner product in this space is written as:

$$\mathrm{Tr}\left[B^\dagger A\right] = \sum_{j,k=1}^{d_S} A_{jk} B_{jk}^* = \langle\langle B\|A\rangle\rangle, \quad \forall A, B \in \mathcal{B}(\mathcal{H}_S), \tag{2.37}$$

where $\langle\langle B\|A\rangle\rangle$ is the standard Euclidean inner product between two vectors in a complex d_S^2-dimensional Hilbert space.

For our purposes, it will be very useful to employ the following identity on the composition of operators in the Liouville space:

$$\begin{aligned}
AB \to \|AB\rangle\rangle &= \sum_{j,k,m=1}^{d_S} A_{jm} B_{mk} |v_j\rangle \otimes |v_k\rangle \\
&= \sum_{k,m=1}^{d_S} B_{mk}(A|v_m\rangle) \otimes |v_k\rangle = A \otimes \mathbb{I}_S \|B\rangle\rangle.
\end{aligned} \tag{2.38}$$

In this way, we have written the composition of the operators A and B as the operator $A \otimes \mathbb{I}_S$ (which lives in the extended Hilbert space $\mathcal{H}_S \otimes \mathcal{H}_S$, i.e., the Liouville space) acting on the vectorized operator $\|B\rangle\rangle$. We can derive an analogous expression for $\|BA\rangle\rangle$:

$$
\begin{aligned}
BA \to \|BA\rangle\rangle &= \sum_{j,k,m=1}^{d_S} B_{jm} A_{mk} |v_j\rangle \otimes |v_k\rangle \\
&= \sum_{j,m=1}^{d_S} B_{jm} |v_j\rangle \otimes (A^T |v_m\rangle) = \mathbb{I}_S \otimes A^T \|B\rangle\rangle.
\end{aligned}
\tag{2.39}
$$

Using these results we can obtain the action of the Liouvillian superoperator $\mathcal{L}$ on $\mathcal{B}(\mathcal{H}_S)$, and in particular on density matrices. By computing $\mathcal{L}\|\rho_S\rangle\rangle$ (with abuse of notation we are representing the Liouvillian as $\mathcal{L}$ both when we consider it as a superoperator and as an operator on the Liouville space) and applying Eqs. (2.38) and (2.39), we can readily observe that the non-diagonal Liouvillian in Eq. (2.28) can be written as an operator acting on $\mathcal{H}_S \otimes \mathcal{H}_S$ as:

$$
\begin{aligned}
\mathcal{L} = &-\frac{i}{\hbar} \left(H \otimes \mathbb{I}_S - \mathbb{I}_S \otimes H^T \right) \\
&+ \sum_{j,k=1}^{D^2-1} \gamma_{jk} \left(F_j \otimes F_k^* - \frac{1}{2}(F_k^\dagger F_j \otimes \mathbb{I}_S + \mathbb{I}_S \otimes (F_k^\dagger F_j)^T) \right).
\end{aligned}
\tag{2.40}
$$

The above equation will be extremely useful for the analytical and/or numerical solution of GKLS master equations. Indeed, we can write the Liouvillian superoperator as a matrix through Eq. (2.40), and then find its eigenvalues and left and right eigenvectors[3]. This procedure is usually called the *spectral analysis* of the Liouvillian, and it is of utmost importance for the study of structured open dynamics [65].

Here, we list some "facts" on the spectral analysis of the Liouvillian, and we refer the interested readers to Refs. [11, 61, 62, 65–68] for more details and proofs. Suppose that we find some eigenvalues and right eigenvectors[4] $\mathcal{L}v_j = \lambda_j v_j$. Then:

- $\lambda_j \in \mathbb{C}$ and $\text{Re}\{\lambda_j\} \leq 0$.

- If $\text{Re}\{\lambda_j\} \neq 0$, then $\text{Tr}[v_j] = 0$.

---

[3]Note that $\mathcal{L}^\dagger \neq \mathcal{L}$, therefore in some cases $\mathcal{L}$ may not be diagonalizable. Moreover, left and right eigenvectors in general do not coincide.

[4]Note that here we are describing the eigenvectors as operators. Of course, we can always switch to the formalism of the Liouville space where the eigenvectors are vectorized via the isomorphism in Eq. (2.36) and viceversa.

- If $\mathcal{L}v_j = \lambda_j v_j$, then $\mathcal{L}v_j^\dagger = \lambda_j^* v_j^\dagger$. In particular, if $v_j^\dagger = v_j$, then $\lambda_j \in \mathbb{R}$. If $\lambda_j \in \mathbb{R}$ and has geometric multiplicity n, then it is always possible to construct n Hermitian right eigenvectors of $\mathcal{L}$ with eigenvalue λ_j.

- Building on the results of the previous point, if $\lambda_j = 0$ and has geometric multiplicity n, then it is always possible to find n properly renormalized density matrices $\rho_k^{(j)}$ such that $\exp(\mathcal{L}t)[\rho_k^{(j)}] = \rho_k^{(j)}$ for all $k = 1, \dots, n$. These density matrices are called the *steady states* of the dynamics.

- If $\dim(\mathcal{H}_S) = d_S < \infty$, then there is always at least one steady state of the dynamics.

- If the steady state ρ_{ss} of the dynamics is unique, then the dynamical semigroup is *relaxing*. That is, $\exp(\mathcal{L}t)[\rho_S] \to \rho_{ss}$ for $t \to \infty$ and for all initial states ρ_S. The search for necessary and sufficient conditions for the uniqueness of the steady state of a quantum dynamical semigroup is still a matter of ongoing research. Some results in this direction have been presented in the past forty years, see for instance the extensive discussion in Ref. [69].

- If there is a right eigenvector v_j such that $\mathrm{Re}\{\lambda_j\} = 0$ but $\mathrm{Im}\{\lambda_j\} \neq 0$, then we say that there are *oscillating coherences* in the dynamics. This is because there will be a subspace of the dynamics where the state of the system will oscillate unitarily also at infinite time without any kind of decay.

We conclude this section by discussing the role of symmetry in the language of the Liouville space. Following the discussion in Sec. 2.4 and Eq. (2.34), we say that there is a weak symmetry of the dynamics if $[\mathcal{L}, \mathcal{U}_g] = 0$, where $\mathcal{U}_g$ is the (superoperator) representation of a symmetry group G. If the latter is a continuous abelian symmetry, we can write it as $\mathcal{U}_g = \exp(ig\mathcal{J})$ for some super-operator $\mathcal{J}$ and $g \in \mathbb{R}$. Then, the weak symmetry reads $[\mathcal{J}, \mathcal{L}] = 0$. Suppose that $\mathcal{J}$ has R known eigenvalues $\{\mu_j\}_{j=1}^R$, each of which has multiplicity n_j ($\mathcal{J}$ is Hermitian, so it is always diagonalizable). Then, we can block-diagonalize the matrix $\mathcal{L}$ given by Eq. (2.40) in the basis of the eigenvectors of $\mathcal{J}$:

$$\mathcal{L} = \bigoplus_{j=1}^R \mathcal{L}_j, \qquad (2.41)$$

where each $\mathcal{L}_j$ is a $n_j \times n_j$ block. In this way, the dimensionality of $\mathcal{L}$ may be highly reduced.

Finally, as discussed in Sec. 2.4 the superoperator $\mathcal{J}$ is associated with a system observable $J \in \mathcal{B}(\mathcal{H}_S)$ via $\mathcal{J} = [J, \cdot]$. In the Liouville space formalism,

this superoperator is straightforwardly written as an operator on $\mathcal{H}_S \otimes \mathcal{H}_S$ through:

$$\mathcal{J} = J \otimes \mathbb{I}_S - \mathbb{I}_S \otimes J^T. \tag{2.42}$$

2.6 Microscopic derivation of the GKLS master equation

In this section we will see how a Markovian master equation can be derived from the microscopic model of an open quantum system coupled to a stationary environment. The general (for simplicity time-independent) Hamiltonian of such a microscopic model can be written as:

$$H = H_S + H_E + \mu H_I, \tag{2.43}$$

where H_S is the system Hamiltonian, H_E is the environment Hamiltonian and H_I is the interaction Hamiltonian between system and environment, while μ is a dimensionless parameter that characterizes the interaction energy.

If we start the dynamics of the overall model in a product state $\rho_{SE}(0) = \rho_S(0) \otimes \rho_E$, then the state of the system at time t will be given by

$$\rho_S(t) = \text{Tr}_E[e^{-iHt}\rho_S(0) \otimes \rho_E e^{iHt}], \tag{2.44}$$

according to Eq. (2.6). As discussed in Sec. 2.1, this evolution can be described through a quantum map for each time t. However, the environment typically has many (or even infinite) degrees of freedom, therefore computing the full evolution driven by $\exp(-iHt)$ is a formidable task. This is why some approximations are necessary in order to obtain a closed (Markovian) form of the quantum map in Eq. (2.44). In particular, we will assume that the coupling between system and environment is *weak*. That is, the interaction Hamiltonian H_I is a perturbation of the total Hamiltonian with $\mu \ll 1$. Physically, this means that the interaction energy is way smaller than the energy of the system, and their ratio is of the order of μ. Let us now see how we can derive a Markovian master equation in the regime of weak coupling.

First, we consider the joint state of the system and environment $\tilde{\rho}_{SE}(t)$, where the tilde indicates that we are working with states (or operators) in the interaction picture [32]. Its dynamics is driven by the following von-Neumann equation:

$$\frac{d}{dt}\tilde{\rho}_{SE}(t) = -\frac{i\mu}{\hbar}[\tilde{H}_I(t), \tilde{\rho}_{SE}(t)], \tag{2.45}$$

where

$$\begin{aligned}
\tilde{\rho}_{SE}(t) &= e^{\frac{i}{\hbar}(H_S+H_E)t}\rho_{SE}(t)e^{-\frac{i}{\hbar}(H_S+H_E)t}, \\
\tilde{H}_I(t) &= e^{\frac{i}{\hbar}(H_S+H_E)t}H_I e^{-\frac{i}{\hbar}(H_S+H_E)t}.
\end{aligned} \tag{2.46}$$

Expanding at the second order in μ the differential equation in Eq. (2.45) (this is the so-called *Born approximation* [8]), we find :

$$\frac{d}{dt}\tilde{\rho}_S(t) = -\frac{\mu^2}{\hbar^2}\int_0^t dt'\,\mathrm{Tr}_E\{[\tilde{H}_I(t),[\tilde{H}_I(t'),\tilde{\rho}_S(t')\otimes\rho_E]\}, \qquad (2.47)$$

where we have assumed $\mathrm{Tr}_E[[\tilde{H}_I(t),\rho_{SE}(0)]] = 0$, which is satisfied by the interaction Hamiltonians of several models of open quantum systems. Let us now decompose the interaction Hamiltonian into system (A_β) and environment (B_β) operators as:

$$\tilde{H}_I(t) = \sum_\beta A_\beta(t)\otimes B_\beta(t). \qquad (2.48)$$

Then, after the change of variable $\tau = t - t'$, we can rewrite Eq. (2.47) as:

$$\frac{d}{dt}\tilde{\rho}_S(t) = -\frac{\mu^2}{\hbar^2}\sum_{\beta,\beta'}\int_0^t d\tau\,\left(\mathcal{B}_{\beta\beta'}(\tau)[A_\beta(t),[A_{\beta'}(t-\tau),\rho_S(t-\tau)]] + H.c.\right),$$

$$(2.49)$$

where we have introduced the autocorrelation functions of the environment:

$$\mathcal{B}_{\beta\beta'}(\tau) = \mathrm{Tr}_E[B_\beta^\dagger(\tau)B_{\beta'}(0)], \qquad (2.50)$$

and we have assumed the stationarity of the state of the environment through $[\rho_E, H_E] = 0$. Under this condition,

$$\mathrm{Tr}_E[B_\beta^\dagger(t)B_{\beta'}(s)] = \mathrm{Tr}_E[B_\beta^\dagger(t-s)B_{\beta'}(0)] = \mathrm{Tr}_E[B_\beta^\dagger(0)B_{\beta'}(s-t)]. \qquad (2.51)$$

We will now perform the so-called *Markov approximation*, which is based on the assumption that the autocorrelation functions of the environment decay very fast in time with respect to the relaxation time of the system. This corresponds to a sort of "fading memory" of the dynamics, so that the state of the system at a given time is not influenced by the states explored at earlier times [8]. This notion resembles the definition of Markovianity we introduced in Eq. (2.24), and indeed we will see that, in many cases, the evolution under this approximation can be described by a quantum dynamical semigroup.

Let us introduce the phenomenological decay time τ_R at which the state reaches the stationary state of the dynamics. Note that $\tau_R \propto \mu^{-2}$ defines the timescale of the evolution of the state of the system in the interaction picture. The same state in the Schrödinger picture evolves with a different timescale since it displays also the fast oscillations driven by the system Hamiltonian H_S. Let us now assume that the autocorrelation functions of the environment decay towards zero with a timescale defined by the environment correlation time τ_E. For instance, let us suppose that $\mathcal{B}_{\beta\beta'}(\tau) \propto e^{-\tau/\tau_E}$. Then, the

Markov approximation requires that $\tau_E \ll \tau_R$. More specifically, we need to introduce a coarse-graining in Eq. (2.49), which is defined by[5] [1, 74]:

$$\exists t^* \text{ such that } \tau_E \ll t^* \ll \tau_R. \tag{2.52}$$

Then, we can make a time average in Eq. (2.49) using the coarse-graining time t^*, and we obtain the *Bloch-Redfield master equation* [8, 75]:

$$\frac{d}{dt}\tilde{\rho}_S(t) = -\frac{\mu^2}{\hbar^2}\sum_{\beta,\beta'}\int_0^\infty d\tau \, \left(\mathcal{B}_{\beta\beta'}(\tau)[A_\beta(t),[A_{\beta'}(t-\tau),\rho_S(t)]] + H.c.\right). \tag{2.53}$$

Note that even if we are using the same notation as before for the state of the system $\tilde{\rho}_S(t)$, more formally this is a new state defined as the time average of the state of the system over a time interval t^*.

At this point, each system operator can be further decomposed into the sum of the *jump operators* $A_\beta(\omega)$:

$$A_\beta(t) = \sum_\omega A_\beta(\omega)e^{-i\omega t}, \qquad A_\beta(\omega) = \sum_{\epsilon'-\epsilon=\hbar\omega} |\epsilon\rangle\langle\epsilon| A_\beta |\epsilon'\rangle\langle\epsilon'|, \tag{2.54}$$

where the states $|\epsilon\rangle$ are the eigenstates of H_S. Then, the Bloch-Redfield master equation can be written as:

$$\begin{aligned}
\frac{d}{dt}\tilde{\rho}_S(t) = \frac{\mu^2}{\hbar^2}\sum_{\beta,\beta'}\sum_{\omega,\omega'}\Big(&e^{i(\omega'-\omega)t}\Gamma_{\beta\beta'}(\omega)\left(A_{\beta'}(\omega)\tilde{\rho}_S(t)A_\beta^\dagger(\omega')\right.\\
&\left.-A_\beta^\dagger(\omega')A_{\beta'}(\omega)\tilde{\rho}_S(t)\right) + H.c.\Big),
\end{aligned} \tag{2.55}$$

where we have defined

$$\Gamma_{\beta\beta'}(\omega) = \int_0^\infty d\tau \, e^{i\omega\tau}\mathcal{B}_{\beta\beta'}(\tau). \tag{2.56}$$

We can now further simplify the expression in Eq. (2.55) by making use of the final approximation in the derivation of a Markovian master equation from the full microscopic model, namely the *secular approximation*. Then, following a similar argument as for the Markov approximation, one can perform an additional coarse-graining average over Eq. (2.55), so as to neglect all the terms rotating with a frequency which is way faster than $1/\tau_R$. Specifically, we eliminate all the terms for which we can find a coarse-graining time t^* such that [1, 74]:

$$\exists t^* \text{ such that } \left|\omega - \omega'\right|^{-1} \ll t^* \ll \tau_R. \tag{2.57}$$

---

[5]For more details about the different definitions of this coarse-graining time and their physical meaning we refer the readers to, for instance, Refs. [70–73].

Let us suppose that this condition is satisfied for all frequencies $\omega' \neq \omega$, so that all cross elements in Eq. (2.55) would be absent. We will call this approximation the *full secular approximation*. Then, the only remaining terms in Eq. (2.55) can be rearranged to obtain the following master equation, where for convenience we have also switched back to the Schrödinger picture [8]:

$$\frac{d}{dt}\rho_S(t) = -\frac{i}{\hbar}[H_S + H_{LS}, \rho_S(t)] + \mathcal{D}[\rho_S(t)], \tag{2.58}$$

where we have introduced the *Lamb-shift Hamiltonian*

$$H_{LS} = \sum_{\omega} \sum_{\beta,\beta'} S_{\beta\beta'}(\omega) A_{\beta}^{\dagger}(\omega) A_{\beta'}(\omega), \tag{2.59}$$

and the *dissipator*

$$\mathcal{D}[\rho_S] = \sum_{\omega} \sum_{\beta,\beta'} \gamma_{\beta\beta'}(\omega) \left(A_{\beta}(\omega)\rho_S A_{\beta'}(\omega)^{\dagger} - \frac{1}{2}\{A_{\beta'}(\omega)^{\dagger} A_{\beta}(\omega), \rho_S\} \right). \tag{2.60}$$

The coefficients are defined by:

$$\begin{aligned} \gamma_{\beta\beta'}(\omega) &= \Gamma_{\beta\beta'}(\omega) + \Gamma_{\beta'\beta}^{*}(\omega), \\ S_{\beta\beta'}(\omega) &= \frac{\Gamma_{\beta\beta'}(\omega) - \Gamma_{\beta'\beta}^{*}(\omega)}{2i}. \end{aligned} \tag{2.61}$$

It can be shown that $H_{LS}^{\dagger} = H_{LS}$ and that the coefficients $\gamma_{\beta\beta'}$ give rise to a positive semi-definite matrix [8]. Therefore, the master equation in Eq. (2.58) is in the GKLS form as in Eq. (2.28), and we have derived a Markovian master equation starting from the full model of an open quantum system coupled to an external environment.

While the well-known derivation we have provided above is based on some physically motivated approximations [8, 11, 74], it is worth pointing out that a rigorous mathematical derivation of the GKLS master equation starting from a complete microscopic model was introduced by Davies in the 70s [76, 77]. The mathematically refined idea of Davies' derivation relies on the so-called Bogolyubov-van Hove limit, characterized by $\mu \to 0$, $t \to \infty$ and $\mu^2 t = \tau =$ const in Eq. (2.49).

2.7 Quantum collision models

In Sec. 2.6 we have shown that a GKLS master equation can be derived starting from the microscopic model of an open quantum system weakly coupled to a stationary environment whose autocorrelation functions decay very fast in time. Here, we will present another scenario in which a Markovian master

equation for the open system only can be obtained from the unitary evolution of a larger physical system. In particular, we will discuss the general aspects of the theory of *collision models*. The interested readers can check the excellent recent review on this topic by Ciccarello et al. for further references and details [78].

The core idea of quantum collision models is to reproduce a non-unitary open system dynamics through repeated "collisions" (i.e., unitary interactions lasting for a timestep Δt) between the open system and some external particles "of the environment", which are usually called *ancillas*. In Markovian collision models, after each collision the colliding ancilla goes away and never interacts again with the system, so that we can forget about it. This corresponds to performing the partial trace on the degrees of freedom of the ancilla after each timestep.

Let us now formalize this idea mathematically. Let us say that the Hilbert space of the system is $\mathcal{H}_S$, while the Hilbert space of jth ancilla is $\mathcal{H}_{E_j}$. Before the collision, we prepare the state of the ancilla in ρ_{E_j}, and we assume that the state of the system is initialized in ρ_S. Then, after the collision with the jth ancilla the state of the system is:

$$\rho_{S,j} = \text{Tr}_{E_j}[U_I(\Delta t)\rho_S \otimes \rho_{E_j}U_I^\dagger(\Delta t)]. \tag{2.62}$$

The unitary operator describing the collision reads:

$$U_I(\Delta t) = \exp\left[-\frac{i}{\hbar}\left(g_S H_S + g_I H_{I,j}\right)\Delta t\right], \tag{2.63}$$

where H_S is the free system Hamiltonian and H_I is the interaction Hamiltonian, which are both dimensionless. The magnitudes of these energies are respectively g_S and g_I.

Let us now suppose that all the ancillas are identical, they are initialized in the same state ρ_E and they collide with the system through the same interaction Hamiltonian H_I. Then, we can introduce a well-defined quantum map $\phi_{\Delta t}$ to describe a generic collision between the system and a single ancilla:

$$\phi_{\Delta t} = \text{Tr}_E[U_I(\Delta t)\cdot\otimes\rho_E U_I^\dagger(\Delta t)], \tag{2.64}$$

where E refers to the degrees of freedom of a single generic ancilla, and U_I is written as in Eq. (2.63) but without the dependency on j. Let us suppose we start the system dynamics in $\rho_S(0)$ and we perform n collisions. Then, the state of the system at the end of this evolution will be given by:

$$\rho_S(n\Delta t) = \phi_{\Delta t}^n[\rho_S(0)]. \tag{2.65}$$

Our aim is to derive a Markovian master equation starting from the action of the quantum map in Eq. (2.64). Note that the expression in Eq. (2.65)

already tells us that the evolution of the state of the system during the jth collision does not depend on the previous history of $\rho_S(t)$, i.e., the Markovianity between the collisions is enforced by construction. Then, what we need is some kind of "smooth" evolution of $\rho_S(j\Delta t)$ to mimic the GKLS dynamics in Eq. (2.29). Quite intuitively, we can obtain this by taking the limit of infinitesimal timestep $\Delta t \to 0^+$.

If Δt is infinitesimal, we can apply the Baker-Campbell-Hausdorff formula to Eq. (2.64) and we obtain:

$$
\begin{aligned}
\phi_{\Delta t}[\rho_S] =& \rho_S - \frac{i}{\hbar}\Delta t\, \mathrm{Tr}_E[[g_S H_S + g_I H_I, \rho_S \otimes \rho_E]] \\
& - \frac{\Delta t^2}{2\hbar^2}\, \mathrm{Tr}_E[[g_S H_S + g_I H_I, [g_S H_S + g_I H_I, \rho_S \otimes \rho_E]]] + O(\Delta t^3).
\end{aligned}
\tag{2.66}
$$

We will now make two fundamental assumptions. The first one is $\mathrm{Tr}_E[[H_I, \rho_S \otimes \rho_E]] = 0$ for all ρ_S. This is always true, for instance, if

$$
H_I = \sum_\beta A_\beta \otimes B_\beta,
\tag{2.67}
$$

similarly as in Eq. (2.48), and all the ancilla operators are such that $\mathrm{Tr}_E[B_\beta \rho_E] = 0$. Note that this requirement is equivalent to the condition we assumed to derive Eq. (2.47) for the full microscopic model in the previous section. The second assumption is $g_S \ll g_I$ (i.e., the magnitude of the collision energy is much larger than the system energy) and $g_I^2 \Delta t/\hbar^2 \to \gamma$, $g_S^2 \Delta t/\hbar^2 \to 0$ for $\Delta t \to 0^+$, where γ is a finite constant with the units of the inverse of time. Under these assumptions, Eq. (2.66) becomes:

$$
\begin{aligned}
\phi_{\Delta t}[\rho_S] =& \rho_S - \frac{i}{\hbar}\Delta t g_S[H_S, \rho_S] + \gamma \Delta t\, \mathrm{Tr}_E[H_I \rho_S \otimes \rho_E H_I - \frac{1}{2}\{H_I^2, \rho_S \otimes \rho_E\}] \\
& + O(g_S^2 \Delta t^2/\hbar^2) + O(g_S g_I \Delta t^2/\hbar^2) + O(\Delta t^3).
\end{aligned}
\tag{2.68}
$$

For a single collision, $\rho_S(t + \Delta t) = \phi_{\Delta t}[\rho_S(t)]$, so:

$$
\begin{aligned}
\frac{d}{dt}\rho_S(t) =& \lim_{\Delta t \to 0^+} \frac{\rho_S(t + \Delta t) - \rho_S(t)}{\Delta t} = \lim_{\Delta t \to 0^+} \frac{\phi_{\Delta t}[\rho_S(t)] - \rho_S(t)}{\Delta t} \\
=& -\frac{i}{\hbar}g_S[H_S, \rho_S(t)] + \gamma \sum_{\beta,\beta'} \mathrm{Tr}_E[B_\beta^\dagger B_{\beta'} \rho_E]\Big(A_{\beta'}\rho_S(t)A_\beta^\dagger \\
& - \frac{1}{2}\{A_\beta^\dagger A_{\beta'}, \rho_S(t)\}\Big),
\end{aligned}
\tag{2.69}
$$

where we have used Eqs. (2.67) and (2.68). It is immediate to see that Eq. (2.69) is in GKLS form, which is what we were looking for. In particular,

we can simulate a quantum dynamical semigroup driven by the Liouvillian $\mathcal{L}$ defined as in Eq. (2.69) at time t by performing n repeated collisions between system and ancillas, with $n = t/\Delta t$. In other words:

$$\exp(\mathcal{L}t) = \lim_{\Delta t \to 0^+} \phi^n_{\Delta t}, \text{ with } n = t/\Delta t. \tag{2.70}$$

Note that, using the same approximations, we could have obtained exactly the same quantum dynamical semigroup also employing this slightly different unitary operator for the collisions: $U_I(\Delta t) = e^{-\frac{i}{\hbar} g_S H_S \Delta t} e^{-\frac{i}{\hbar} g_I H_I \Delta t}$. That is, we can first perform the collision and then, independently, the free system evolution. This allows us to tune g_I and g_S by using different collision timesteps.

The derivation of the GKLS master equation associated with a Markovian collision model we have provided above follows the lines of different works published in the last ten years [5, 79–81]. The quantum collision models are employed for disparate tasks in which open quantum systems play a relevant role. To name just a few, they are employed to study the problem of thermalization or "homogenization" of the open system [82, 83], to analyze the non-Markovianity of the open evolution, either through collisions between the system and some ancillas that are correlated with the previous ones [84, 85] or through a Markovian embedding of pseudomodes to generate a non-Markovian dynamics [81], and to study the elementary variations of heat, work and energy in quantum thermodynamics [86–88]. Moreover, the fact that collision models are based on the application of repeated simple unitaries makes them very convenient to be implemented on quantum computers, so as to quantum simulate the GKLS dynamics we are interested in. Further discussions can be found in Refs. [78, 89].

Chapter 3

Applications to multipartite open quantum systems

3.1 A Markovian master equation for multipartite open quantum systems and its properties

In Sec. 2.6 we have shown how a Markovian master equation can be derived from a general microscopic model of an open quantum system weakly coupled to an environment. Here, we will discuss some issues that arise in this derivation if the open system is multipartite, how to overcome them, and what are the properties of the master equation we will obtain.

3.1.1 Global and local master equations

Let us suppose that the open system is multipartite and is composed of M subsystems. The system Hamiltonian, in general, includes some local terms (acting on a single subsystem only) and the interaction between the subsystems:

$$H_S = H_{S,L} + \lambda H_{S,I} = \sum_{j=1}^{M} H_{S,j} + \lambda H_{S,I}, \qquad (3.1)$$

where $H_{S,L}$ contains all the local terms, while $H_{S,I}$ is the inter-subsystem interaction term. λ is the dimensionless coupling constant that characterizes the magnitude of these interactions.

Let us go back to the derivation of the microscopic GKLS master equation. Getting the form of the Bloch-Redfield master equation in Eq. (2.55) requires introducing the jump operators in Eq. (2.54). To do so, we must find the eigenvalues and eigenvectors of the system Hamiltonian H_S. For convenience,

we will term these as the "global eigenvectors" and "global eigenvalues":

$$H_S = \sum_{k=1}^{d_S} E_k^{(g)} \left| e_k^{(g)} \right\rangle \left\langle e_k^{(g)} \right|, \tag{3.2}$$

where we recall that d_S is the dimension of the system Hilbert space. If the system is multipartite and/or a many-body quantum system, then it might be difficult to find the diagonalization in Eq. (3.2). For this reason, a "local approach" can be invoked, which makes use of the "local eigenvalues" and "local eigenvectors" of the local Hamiltonian $H_{S,L}$:

$$H_{S,L} = \sum_{k=1}^{d_S} E_k^{(l)} \left| e_k^{(l)} \right\rangle \left\langle e_k^{(l)} \right|. \tag{3.3}$$

It is much easier to perform this diagonalization, as the eigenvectors $\{\left| e_k^{(l)} \right\rangle\}_{k=1}^{d_S}$ are given by the tensor product of the local bases of each $H_{S,j}$. Two different approaches are then adopted in the literature:

Global master equation The so-called *global master equation* is the standard Bloch-Redfield master equation in Eq. (2.55), typically with the application of the secular approximation. The jump operators of the global master equation are derived from the diagonalization of the full system Hamiltonian as in Eq. (3.2).

Local master equation The *local master equation* is derived under an additional approximation on the "locality" of its jump operators. Specifically, it is a Bloch-Redfield equation (typically with secular approximation) where the jump operators are the ones obtained with the local system Hamiltonian in Eq. (3.3). This means that the interaction term $H_{S,I}$ is neglected during the derivation of the master equation, and it appears only in the effective system Hamiltonian H_S of the final GKLS master equation in Eq. (2.58).

The local master equation is widely adopted in the literature, especially in the field of open many-body quantum systems. However, its validity has been disputed in a number of works. In particular, few years ago Levy and Kosloff showed that the local master equation leads to a violation of the second law of thermodynamics in a simple system of two coupled qubits interacting with two baths at different temperature [26]. In 2016, Trusheckhin and Volovich carefully analyzed the conditions for the validity of the local approximation, and by employing matrix perturbation methods they showed that the local master equation is valid whenever $\lambda \ll 1$, and the error of this approximation with respect to the global master equation is of the order of $O(\lambda)$ [27] (if the

system energies are degenerate then a more careful discussion is necessary). Then, the violation of the second law found in Ref. [26] is due to an error of order $O(\lambda)$, therefore the local master equation can still be employed for thermodynamic studies in a limited regime of parameters, taking this error into account. Physically, the requirement $\lambda \ll 1$ corresponds to the subsystem energies in each $H_{S,j}$ being much larger than the magnitude of the subsystem-subsystem interaction.

Several comparisons between the local and global master equations have been presented, and Publication **I** briefly reviews them. Although the local master equation is obtained via an additional approximation applied to the global master equation, in the literature we can often find the claim that the global master equation may fail in regimes of validity where the local master equation is valid [28, 29]. This is due to the fact that many references in the literature use the term "global master equation" to refer to the more specific "global master equation under the full secular approximation", i.e., a Bloch-Redfield master equation derived using the global jump operators according to Eq. (3.2) and where all the terms with $\omega' \neq \omega$ are neglected in Eq. (2.55). We see that two different features of the microscopic master equation are taken into account at once here. Therefore, care must be taken when talking about the "global master equation".

A global master equation with a consistent secular approximation is therefore a better approximation than a local one, by construction. Still, an indiscriminate application of the full secular approximation can fail. Let us show with an example why some issues with the global master equation in full secular approximation arise for multipartite open quantum systems. For a single quantum system, the energy levels are usually equally spaced (e.g., in a harmonic oscillator), or the gap between the levels is considerably different between different pairs of levels. As a consequence, the frequencies in Eq. (2.55) are either equal ($\omega = \omega'$, so that the corresponding terms are not removed by the full secular approximation) or very different, and in the latter case they can be safely removed through the full secular approximation according to Eq. (2.57). This is in general not true for a multipartite system. For instance, consider the case of two coupled qubits that are slightly detuned. The system Hamiltonian can be written as:

$$H_S = \frac{\hbar\omega_1}{2}\sigma_1^z + \frac{\hbar\omega_2}{2}\sigma_2^z + \lambda(\sigma_1^+\sigma_2^- + H.c.). \qquad (3.4)$$

If $\Delta = \frac{|\omega_1 - \omega_2|}{\omega_1}$ is small (we assume that the order of magnitude of the qubit frequencies is the same), that is, $\Delta \ll 1$, and $\lambda \ll 1$ as well, then the gap between the second and the third energy level of this Hamiltonian is small

compared to the qubit energies. More specifically, the eigenvalues of H_S are:

$$E_0 = -\frac{\hbar(\omega_1 + \omega_2)}{2}, \qquad E_1 = -\sqrt{\lambda^2 + \hbar(\omega_1 - \omega_2)^2/4},$$
$$E_2 = -E_1, \qquad E_3 = -E_0. \tag{3.5}$$

Then, a jump frequency in Eq. (2.55) can be $\omega = E_1 - E_0$, while another one can be $\omega' = E_2 - E_0$. Clearly, $\omega - \omega' = E_1 - E_2$, which is small compared to the qubit energies. Therefore, the full secular approximation cannot be applied to these terms because the condition in Eq. (2.57) is not satisfied. Increasing the number of subsystems, we find more and more scenarios with energy gaps for which the full secular approximation cannot be applied, if the coupling between the subsystems is small. Note that $\lambda \ll 1$ is at the same time the sufficient condition for the validity of the local approximation and the necessary condition for the breaking of the global master equation with full secular approximation. This is why it is often claimed in the literature that in this regime the local approach is better than the global one [28, 29].

The aim of Publication **I** is to review the literature on the "local vs global problem" and to shed light on its subtlest aspects. In particular, Publication **I** shows that the global master equation (as we have defined it above) is *always* valid under the regime of validity of the Bloch-Redfield master equation (i.e., under the Born and Markov approximations) if the secular approximation is applied in a correct way. That is, if we remove only the terms with frequencies ω, ω' in Eq. (2.55) that satisfy the condition in Eq. (2.57). This approximation is usually called *partial secular approximation* [72, 90]. Remarkably, Redfield himself made a comment on the possibility of performing this approximation in his seminal paper [75].

Let us say that the frequencies that are not eliminated by the partial secular approximation can be written as the elements of a set $(\omega, \omega') \in \mathsf{PSA}$. Then, the global master equation under the partial secular approximation can be written as Eq. (2.58), that is, $\mathcal{L}[\rho_S(t)] = -i/\hbar[H_S + H_{LS}, \rho_S(t)] + \mathcal{D}[\rho_S(t)]$, with Lamb-shift Hamiltonian given by

$$H_{LS} = \sum_{\beta,\beta'} \sum_{(\omega,\omega') \in \mathsf{PSA}} S_{\beta,\beta'}(\omega, \omega') A_\beta^\dagger(\omega') A_{\beta'}(\omega), \tag{3.6}$$

and dissipator

$$\mathcal{D}[\rho_S] = \sum_{\beta,\beta'} \sum_{(\omega,\omega') \in \mathsf{PSA}} \gamma_{\beta,\beta'}(\omega, \omega') \left(A_{\beta'}(\omega) \rho_S A_\beta^\dagger(\omega') - \frac{1}{2}\{A_\beta^\dagger(\omega') A_{\beta'}(\omega), \rho_S\} \right). \tag{3.7}$$

The jump operators are defined in Eq. (2.54) according to the total system

Hamiltonian decomposed as in Eq. (3.2), while the coefficients are:

$$\gamma_{\beta\beta'}(\omega, \omega') = \Gamma_{\beta\beta'}(\omega) + \Gamma^*_{\beta'\beta}(\omega'),$$

$$S_{\beta\beta'}(\omega, \omega') = \frac{\Gamma_{\beta\beta'}(\omega) - \Gamma^*_{\beta'\beta}(\omega')}{2i}, \tag{3.8}$$

where $\Gamma_{\beta\beta'}(\omega)$ is defined in Eq. (2.56).

Publication **I** discusses how the global master equation with partial secular approximation introduced above is accurate in all regimes of validity of the Bloch-Redfield master equation. In particular, this master equation is valid also when $\lambda \ll 1$ (despite being "global"), where it gives the same physical predictions as the local equation. Viceversa, if $\lambda \gg 1$ then the full secular approximation is typically valid, and the predictions given by the global master equation with either full or partial secular approximation coincide. Therefore, the global master equation with partial secular approximation can be considered as an "always-valid" bridge between the local master equation and the global master equation with full secular approximation. This idea has been further analyzed in a recent work [91]. Moreover, Publication **I** discusses the regimes of validity of the local and full-secular master equations in the presence of common or separate baths, and their consequences for the observation of physical effects such as entanglement generation, quantum beats, and steady-state heat current. We refer the reader to the original paper for further details, while further developments on the local vs global problem after the appearance of Publication **I** can be found, for instance, in Refs. [91–95].

A common concern on the global master equation with partial secular approximation is the fact that, being derived from the Redfield equation without the full secular approximation, it might not yield a completely positive dynamics. This is a typical issue of the Bloch-Redfield equation [96]. We can answer this criticism in two different ways. First, it has been recently shown that some sufficient conditions for the complete positivity of the master equation with partial secular approximation can be derived under reasonable assumptions [71, 72]. This makes sense, as the terms leading to the breaking of complete positivity in the Redfield equation are typically the fast-oscillating ones, which are still eliminated by the partial secular. Secondly, we may adopt a different vision toward the issue of the complete positivity of the master equation: the exact reduced dynamics in Eq. (2.44) is completely positive. Starting from that equation, we have applied i) the Born approximation ii) the Markov approximation, and doing this we obtain the Redfield equation. If the latter is not completely positive, then the errors due to negativity issues must be within the accuracy of these approximations. If we further apply the secular approximation, we may recover mathematically a completely positive dynamics, but we are not improving the accuracy of the master equation. Therefore,

we may also work with a non-completely positive master equation, if we know that there may be negativity issues of the order of the Born-Markov approximation. This idea has been extensively discussed and analyzed by Hartmann and Strunz, who showed that, for the sake of numerical simulations, the Bloch-Redfield equation is the most accurate weak-coupling master equation despite its lack of complete positivity [97], and it typically provides better predictions than master equations with full secular approximation. If we observe a considerable violation of the positivity in the dynamics predicted by our Redfield (or partial secular) master equation, then this is a sign that the conditions for the Born-Markov approximations are breaking down, and we need to rely on better numerical methods. Curing these negativities via the full secular approximation, indeed, would only lead to a mathematically well-defined master equation that is not reproducing anymore the evolution of the microscopic model of our interest. Similar considerations can be found also in Ref. [98].

Finally, inspired also by the results in Publication **I** and related discussions on the partial secular approximation, A. Trusheckhin has introduced the "Unified GKLS master equation" [99]. This equation can be thought of as the mathematical formalization of the global master equation with partial secular approximation, which can be written in GKLS form and thus is completely positive. The core idea of the unified master equation is to assume that the system Hamiltonian can be written as $H_S = H_S^{(0)} + \mu^2 \delta H_S$, where $[H_S^{(0)}, \delta H_S] = 0$ and μ is the system–environment coupling constant. The energy levels of $H_S^{(0)}$ are either well-separated or fully degenerate (so that this term could be well-treated through the full secular approximation), while the term δH_S introduces some quasi-degeneracies in the energy levels (i.e., the small energy gaps that need the partial secular approximation). Then, a microscopic GKLS master equation is derived following Davies' approach [76, 77] based on the rigorous Bogolyubov-van Hove limit, and the terms that are not deleted by the partial secular approximation are preserved in this equation as well. The coefficients of the master equation are slightly modified, such that, for instance, $\gamma_{\beta\beta'}(\omega, \omega')$ in Eq. (3.8) becomes a new $\gamma_{\beta\beta'}(\bar{\omega})$ that is evaluated at the average frequency $\bar{\omega} = (\omega + \omega')/2$ (this idea was sketched also in Refs. [98, 100]). By doing so, it can be shown that the master equation is in GKLS form. The unified master equation has the nice feature of being completely positive, and therefore it generates a mathematically well-defined quantum dynamical semigroup. However, following the reasoning in Ref. [97], for the sake of precision of the numerical simulations it is slightly less accurate than the standard master equation in partial secular approximation we presented above.

To conclude, we have shown that a careful derivation of the microscopic master equation that makes use of the partial secular approximation provides

us with a general Markovian equation to study multipartite open quantum systems. This equation is particularly convenient for the numerical simulations, and if it happens not to be in GKLS form, then it can always be brought into this form by following the procedure in Ref. [99].

3.1.2 Symmetries of the master equation under the full and partial secular approximation

Publication **II** shows that the global master equation with partial secular approximation has a weak symmetry under quite general conditions. Suppose that the system Hamiltonian can be written as a collection of M bosonic and/or fermionic modes, such as:

$$H_S = \sum_{k=1}^{M} E_k a_k^\dagger a_k, \qquad (3.9)$$

where E_k are the energies of the eigenmodes and a_k is a bosonic or fermionic annihilation operator. General quadratic Hamiltonians can be brought into this form by means of Bogolyubov transformations. Then, let us introduce the total-number-of-particles operator as:

$$N = \sum_{k=1}^{M} a_k^\dagger a_k. \qquad (3.10)$$

This operator generates the one-parameter group of operators

$$U(g) = \exp(igN), \qquad g \in \mathbb{R}. \qquad (3.11)$$

Analogously, we can define the one-parameter group of superoperators

$$\mathcal{U}_g = \exp(ig\mathcal{N}), \qquad g \in \mathbb{R}, \qquad (3.12)$$

generated by the total-number-of-particles superoperator $\mathcal{N} = [N, \cdot]$. In the Liouville space, this superoperator is written as $N \otimes \mathbb{I}_S - \mathbb{I}_S \otimes N^T$, according to Eq. (2.42).

Now, let us suppose that we derive a GKLS global master equation with partial secular approximation starting from a very general microscopic model of the system with Hamiltonian H_S coupled to an environment. Let us say that we are able to introduce a well-defined Liouvillian $\mathcal{L}$ associated with this master equation. Then, Publication **II** proves that, under some broadly valid conditions for which we refer to the original article, the semigroup generated by $\mathcal{L}$ is covariant under the action of the above-defined $\mathcal{U}_g$. That is, the partial secular master equation displays the weak symmetry

$$\mathcal{U}_g e^{\mathcal{L}t} \mathcal{U}_g^\dagger = e^{\mathcal{L}t}, \quad \forall g \in \mathbb{R}, \forall t, \quad \text{or equivalently } [\mathcal{L}, \mathcal{N}] = 0. \qquad (3.13)$$

We remind that, in general, no conserved quantity N is associated with this weak symmetry, as discussed in Sec. 2.4. Still, this symmetry has remarkable consequences. Indeed, first of all we can block-diagonalize the Liouvillian with the eigenvectors of $\mathcal{N}$ (which can be trivially found), as discussed in Sec. 2.5 and according to Eq. (2.41). In particular, we can write $\mathcal{L}$ in the Liouville space as:

$$\mathcal{L} = \bigoplus_j \mathcal{L}_j, \tag{3.14}$$

where $\mathcal{L}_j$ acts on the eigenvectors of $\mathcal{N}$ with eigenvalue j. Note that these eigenvectors written as operators are such that the difference between the total number of particles in the ket and the total number of particles in the bra is equal to j. For instance, let us consider the case of two fermionic modes. Then, the operator $|01\rangle\langle00|$ is an eigenvector of $\mathcal{N}$ with eigenvalue 1; $|00\rangle\langle00|$ and $|11\rangle\langle11|$ are eigenvectors of $\mathcal{N}$ with eigenvalue 0, and so on. Moreover, Publication **II** shows that $\mathcal{L}_{-j} = \mathcal{L}_j^*$.

Another fundamental result of Publication **II** is the fact that, if the steady state of the dynamics is unique, then it must be a linear combination of eigenvectors of $\mathcal{N}$ with eigenvalue 0. That is, to find it we only need to analyze the block $\mathcal{L}_0$ of the Liouvillian. Clearly, these results provide us with a remarkable dimensionality reduction for both the problem of finding the steady state of the dynamics and of solving the full time evolution. We will see in Sec. 3.3 further applications of these findings.

Dimensionality reduction is not the only consequence of this covariance of the master equation. It has been shown that global master equations with the full secular approximation satisfy a different kind of covariance, whose group of operators is generated by the system Hamiltonian H_S [57, 101], and not by N. Publication **II** shows that for the partial secular approximation this is not true. This finding, derived from the microscopic model, is in contrast with different results based on a derivation of the dynamics from general thermodynamic principles, which claim that any open dynamics that satisfies the laws of weak-coupling thermodynamics must be covariant under the group of operators generated by H_S [30]. Therefore, we see how our result brings a relevant contribution to a discussion on the foundations of quantum thermodynamics (microscopic dynamics vs general principles) that, to the best of our knowledge, has not been settled yet. For instance, the property $[\mathcal{L}, \mathcal{N}] = 0$ implies that the steady state of the dynamics can have coherences in the eigenbasis of H_S. These coherences, however, must be eigenvectors of $\mathcal{N}$ with eigenvalue 0 (e.g., $|01\rangle\langle10|$ for two fermions).

3.2 Analog simulation of open quantum systems in circuit QED

Publication **III** reviews and derives different results on *dissipation engineering* in the field of circuit quantum electrodynamics (circuit QED). That is, how we can reproduce and tune the action of external environments on superconducting qubits; this is usually referred to as "analog quantum simulation of open quantum systems". More specifically, Publication **III** analyzes in detail how we can mimic the action of *thermal baths* by inserting resistive elements in the superconducting circuit. This study has been inspired by some experimental works conducted at Aalto University that showed how these resistive elements can be engineered in a superconducting chip so as to study different phenomena in quantum thermodynamics [102–104].

Reviewing the theory of circuit QED goes way beyond the scope of this chapter. We refer the interested readers either to the discussions in Publication **III** and to some excellent recent reviews on this topic [105–107]. Therefore, in this section we will just briefly present in a discursive way the main results of Publication **III** and the general idea behind them.

The degrees of freedom that are typically quantized in circuit QED are the fluxes of the branches of a superconducting circuit and their conjugate momenta. The flux of a circuit branch at time t is defined as:

$$\varphi(t) = \int_{-\infty}^{t} V(t')dt', \tag{3.15}$$

where $V(t)$ is the voltage difference across this branch. Let us now analyze a very simple superconducting circuit composed of a superconducting qubit (more specifically a transmon qubit [107]) coupled to a resistor through a capacitor, as in Fig. 3.1. The degrees of freedom we are interested in are the flux φ_A associated with the transmon qubit "A" and the flux φ_R associated with the resistor, and their corresponding conjugate momenta. The branches associated with the fluxes are the parts of circuits that go from the ground at the bottom of each circuit branch to the black dot at the top. That is, we need to consider the voltage difference across the transmon qubit to find φ_A and across the resistor to find φ_R. The coupling capacitor C_g makes the transmon qubit and the resistor interact.

Publication **III** discusses how to obtain the total Hamiltonian of the superconducting circuit in Fig. 3.1. This is not a trivial task, because the resistor is a dissipative element and is not well-described through the standard formalism of circuit QED. To formalize the Hamiltonian of the resistor, Publication **III** makes use of the so-called Foster's decomposition of a resistor as an infinite set of LC circuits, which was introduced by Devoret [108]. In this way, an excitation coming from the qubit may "travel" forever along the set of LC circuits of
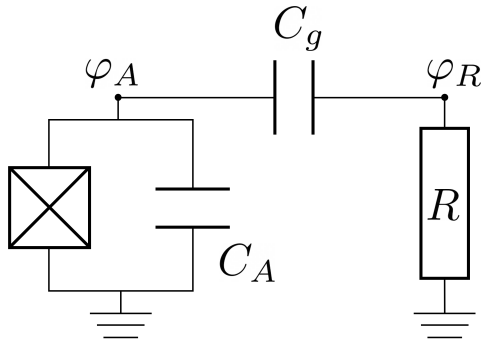
Figure 3.1: A transmon qubit with internal capacitance C_A and flux φ_A capacitively coupled to a resistor.

the resistor without ever coming back. This effect, which is due to the infinite number of LC circuits, mimics the emergence of dissipation, and can be formalized mathematically through the Sokhotski–Plemelj theorem, as explained in Publication **III**. This procedure, however, is not enough to obtain the final Hamiltonian of the superconducting circuit. Indeed, the standard procedure to do so in circuit QED starts from the circuit Lagrangian, which can be obtained relatively trivially by looking at the network of the circuit nodes [107, 108], and then derives the Hamiltonian by applying the Legendre transform. This is not easy, because it can be shown that it corresponds to inverting an infinite-dimensional matrix. To accomplish this task, Publication **III** relies on some theoretical methods recently developed by Parra-Rodriguez et al. [109, 110]. By applying these results and assuming the weak coupling limit, which reads $C_g \ll C_A$ (coupling capacitance much smaller than the internal capacitance of the qubit), we are able to find the final Hamiltonian of the circuit in Fig. 3.1.

The final Hamiltonian we obtain for the circuit in Fig. 3.1 is the standard Hamiltonian of the dissipative spin-boson model [8], where a single qubit is weakly coupled through σ_x to a stationary thermal bath. Moreover, our results show that the spectral density of this bath is Ohmic, which is coherent with the fact that the voltage fluctuations across the resistor emit Johnson-Nyquist thermal noise. Since the spectral density is Ohmic, under reasonable assumptions[1] the dynamics of the transmon qubit is Markovian, and can be described through a simple GKLS master equation (we refer the readers to the original article for its form and details).

Remarkably, Publication **III** shows that we can simulate also some multi-partite open quantum systems through similar superconducting circuits that

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[1]More specifically, we must assume weak coupling between qubit and resistor, and that $k_B T \gg \hbar/\tau_R$, where T is the resistor temperature, and τ_R is the relaxation time of the qubit, to guarantee a Markovian dynamics [8].
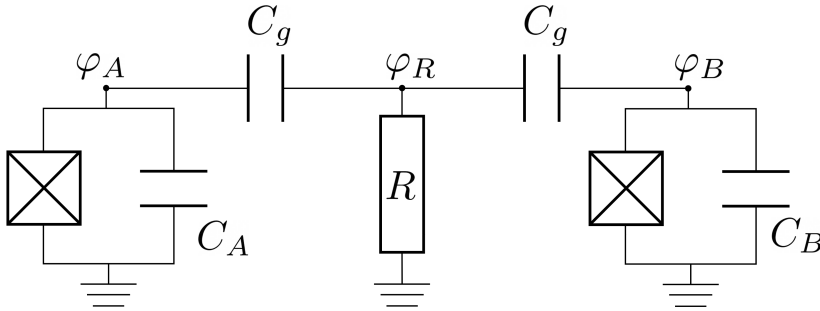
Figure 3.2: Two transmon qubits with internal capacitances C_A and C_B are coupled to a common resistor with resistance R through two coupling capacitors that, for simplicity, have the same capacitance C_g.

contain resistors. In particular, the circuit in Fig. 3.2 depicts two transmon qubits ("A" and "B") capacitively coupled to the same resistor R. By employing the same methods as for a single transmon qubit (including the weak coupling limit that now is given by $C_g \ll C_A, C_B$), we are able to derive the circuit Hamiltonian, which is the Hamiltonian of two non-interacting qubits weakly coupled to a thermal bath. A direct coupling between the qubits can be inserted as well. The master equation that can be derived for the dynamics of the qubits only is the global master equation for two spins in a common bath that is discussed in Publication **I**.

Finally, Fig. 3.3 displays two transmon qubits that are directly coupled through a capacitor C_c, while the qubit B is also coupled to a resistor R. Publication **III** shows that, if we assume the weak coupling limit for both the qubit-qubit and the qubit-resistor capacitors, that is, $C_c \ll C_A, C_B$ and $C_g \ll C_A, C_B$, then the circuit Hamiltonian we can derive describes two weakly interacting qubits, one of which is also weakly coupled to a thermal bath. Therefore, in this scenario there is a "local" (or "separate") bath acting on a single qubit only. Since the coupling between the qubits is weak, their dynamics is well-described by a local master equation that is discussed in Publication **I**. Note that, due to the structure of the capacitive interaction in circuit QED, we are forced to assume that the qubit-qubit interaction is weak if we want to obtain a local bath. Otherwise, the resistor R would be directly coupled also to the qubit A in the circuit Hamiltonian, despite being coupled only to the qubit B in the circuit network of Fig. 3.3.

In conclusion, Publication **III** shows that circuit QED is an excellent platform to study the dynamics of the simplest examples of multipartite open quantum systems. Some experimental works at Aalto University [102–104] prove that we already have the technology for the experimental investigation
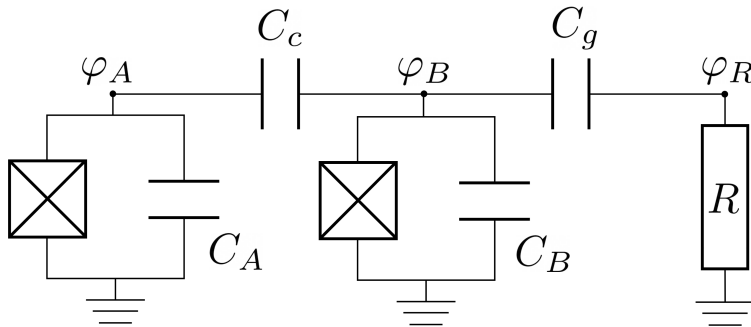
Figure 3.3: Two transmon qubits are coupled through a capacitor with capacitance C_c. Moreover, the qubit B is also coupled to a resistor R through a capacitor with capacitance C_g.

of multipartite Markovian master equations with Ohmic spectral density by inserting resistive elements in the superconducting circuit.

3.3   Spectral analysis for collective phenomena in open quantum systems

Multipartite open quantum systems can display *collective phenomena* due to the coherent interference of the emissions of the open subsystems into the environment, which would not be possible during the local decay of an isolated subsystem only. In this section, we will consider three topical collective effects that are discussed in Publication **IV**, namely *quantum synchronization*, *subradiance* and *entanglement generation*. Let us introduce them.

For simplicity, we will consider an open quantum system made of two subsystems only. Generalizations of these collective effects to more subsystems are possible, although perhaps not trivial. We will start to discuss quantum synchronization [24]. In this thesis, we refer to "quantum synchronization" as the synchronization in time of the oscillations of the mean values of some local observables of the two open subsystems. Synchronization is a paradigmatic phenomenon in Physics and can be induced by dissipation on the system. In our scenario, synchronization is indeed caused by a dissipative bath acting collectively on the subsystems. We point out that different definitions of quantum synchronization can be found in the literature [111].

Superradiance is a well-known phenomenon that was introduced theoretically by Dicke in 1954 [20] and has been studied experimentally since the 70s [21]. It consists in the enhanced (i.e., faster) decay of a bunch of atoms that emit coherently into a common environment. It can be observed when the system is prepared in the so-called *superradiant state*. In contrast, Publica-

tion **IV** focuses on subradiance, which is a complementary phenomenon that emerges in the exactly same physical system as superradiance, but preparing a different initial state, termed *subradiant state* [23]. Subradiance consists in an atomic decay that is slower than in the case of local isolated atoms, and it is due to the negative interference of their emissions into the common environment. Perfect subradiance corresponds to a zero decay rate, i.e., the emission is inhibited and the dynamics lives in a decoherence-free subspace.

Finally, entanglement generation is simply the emergence of entanglement between subsystems that were initially separable. It has been shown that a collective environment can generate entanglement between non-interacting qubits [112, 113].

Publication **IV** considers a system of two slightly detuned non-interacting qubits that are immersed into a common thermal environment, and studies how and under which conditions the above-defined collective phenomena emerge during the open dynamics. It explores a wide range of model parameters and, moreover, it focuses on the physical system of two transmon qubits coupled to a common resistor that has been studied in Publication **III**. This circuit scheme is discussed in the previous section and is depicted in Fig. 3.2. The master equation for the two-qubit dynamics is taken from Publication **I**, and it is written as:

$$
\mathcal{L}[\rho_S(t)] = -\frac{i}{\hbar}[H_S + H_{LS}, \rho_S(t)] + \sum_{j,k=1,2} \gamma_{jk}^{\downarrow} \left(\sigma_j^- \rho_S(t)\sigma_k^+ - \frac{1}{2}\{\sigma_k^+ \sigma_j^-, \rho_S(t)\} \right)
$$
$$
+ \sum_{j,k=1,2} \gamma_{jk}^{\uparrow} \left(\sigma_j^+ \rho_S(t)\sigma_k^- - \frac{1}{2}\{\sigma_k^- \sigma_j^+, \rho_S(t)\} \right).
$$

$$(3.16)$$

$H_S = \hbar\omega_1\sigma_1^z/2 + \hbar\omega_2\sigma_2^z/2$ is the system Hamiltonian (the qubit frequencies are ω_1 and ω_2). σ_1^- is the operator that destroys an excitation in the first qubit, and analogously for σ_2^-. H_{LS} is a Lamb-shift Hamiltonian introducing a spin coupling effect of the form $s_{12}\sigma_1^-\sigma_2^+ + H.c.$ (s_{12} is a temperature-dependent complex coefficient), while $\gamma_{jk}^{\downarrow}$ and $\gamma_{jk}^{\uparrow}$ are coefficients that depend on the bath temperature. We refer the readers to the original article for their detailed expressions.

The master equation in Eq. (3.16) is a global master equation with partial secular approximation. Therefore, it satisfies the symmetry discussed in Publication **II** and Sec. 3.1.2. Specifically, $[\mathcal{L}, \mathcal{N}] = 0$, with $\mathcal{N} = [N, \cdot]$ and $N = |1\rangle\langle 1| \otimes \mathbb{I} + \mathbb{I} \otimes |1\rangle\langle 1|$, where $|1\rangle$ is the excited state of a qubit. As a consequence, we can diagonalize the Liouvillian using the eigenvectors of $\mathcal{N}$, which are trivial to be found.

Let us go back to the collective phenomena we want to observe in the dynamics driven by Eq. (3.16). In particular, our aim is to observe the syn-

chronization of the mean values $\langle\sigma_1^x(t)\rangle$ and $\langle\sigma_2^x(t)\rangle$, that is, of the qubit coherences. If the qubits were free, these mean values would oscillate at their respective frequency ω_1 or ω_2. In the presence of the common bath, however, these observables can synchronize. Let us understand why. First of all, it can be shown that the dynamics of $\langle\sigma_1^x(t)\rangle$ and $\langle\sigma_2^x(t)\rangle$ "live" in the space of the eigenvectors of $\mathcal{N}$ with eigenvalues 1 and -1 only. Moreover, $\mathcal{L}_{-1} = \mathcal{L}_1^*$, therefore we can focus on the block $\mathcal{L}_1$ only. This is a great simplification, because $\mathcal{L}$ is a 16×16 matrix in the Liouville space, while $\mathcal{L}_1$ is a 4×4 matrix. Now, let us say that the eigenvalues of $\mathcal{L}_1$ are $\{\lambda_j^{(1)}\}_{j=1}^4$. Then, the mean values can be written as:

$$\langle\sigma_k^x(t)\rangle = \sum_{j=1}^4 c_{jk}^{(1)} e^{\mathrm{Re}[\lambda_j^{(1)}]t} \cos\left(\mathrm{Im}[\lambda_j^{(1)}]t + \varphi_{jk}^{(1)}\right). \tag{3.17}$$

$c_{jk}^{(1)}$ and $\varphi_{jk}^{(1)}$ depend on the eigenvectors of $\mathcal{L}_1$, on the initial conditions of the dynamics, and on the selected qubit. The time dependence in Eq. (3.17) is quite peculiar: an exponential decay is driven by the real part of the eigenvalues of $\mathcal{L}_1$, while we also observe an oscillatory behavior with a frequency given by the corresponding imaginary part of the eigenvalues. We are now ready to understand how synchronization can emerge in such a system.

Suppose that $\left|\mathrm{Re}[\lambda_1^{(1)}]\right| \leq \left|\mathrm{Re}[\lambda_2^{(1)}]\right| \leq \left|\mathrm{Re}[\lambda_3^{(1)}]\right| \leq \left|\mathrm{Re}[\lambda_4^{(1)}]\right|$, then we define the *spectral gap* as

$$\Delta_1 = \left|\mathrm{Re}[\lambda_2^{(1)}]\right| - \left|\mathrm{Re}[\lambda_1^{(1)}]\right|. \tag{3.18}$$

The real parts of the eigenvalues describe how fast the spectral modes in Eq. (3.17) decay during the dynamics. Therefore, the quantity $1/\left|\mathrm{Re}[\lambda_1^{(1)}]\right|$ defines the *relaxation time* of the coherences, i.e., the time at which the last oscillations of the coherences vanish. Now, suppose there is a large spectral gap between the two smallest (in absolute value) real parts of the eigenvalues in comparison with the relaxation time:

$$\frac{\Delta_1}{\left|\mathrm{Re}[\lambda_1^{(1)}]\right|} > 1. \tag{3.19}$$

Then, intuitively there is a transient time of the dynamics (after the mode driven by $\lambda_2^{(1)}$ has died) during which the oscillations driven by $\lambda_1^{(1)}$ are still alive and there are no other modes in the system dynamics. That is, both qubits are synchronized and oscillate with the same frequency equal to $\mathrm{Im}[\lambda_1^{(1)}]$. Due to the transient character of the synchronization, which eventually will disappear after the relaxation time, this phenomenon is also called "transient quantum synchronization" [24]. Based on these considerations and further

analyses on the structure of the eigenvectors of $\mathcal{L}_1$, Publication **IV** introduces a general measure of transient quantum synchronization.

Subradiance can be treated in a similar way as quantum synchronization. The key difference lies in the fact that the mean values of the observables that describe subradiance (i.e., the qubit energies $\sigma_1^z(t)$ and $\sigma_2^z(t)$) "live" in the block $\mathcal{L}_0$ only. Therefore, to study subradiance we only need to diagonalize a 6×6 matrix. Then, the emergence of a slowly decaying subspace of the dynamics can be related to the presence of a large spectral gap in $\mathcal{L}_0$, as in Eqs. (3.18) and (3.19). Building on these considerations, Publication **IV** puts forward a general measure of subradiance in the open dynamics.

Finally, the emergence of entanglement between the qubits is captured by a figure of merit called *negativity*, which is a well-defined entanglement monotone [114]. The maximum value of the negativity during the dynamics is chosen to characterize entanglement generation. Unfortunately, the negativity cannot be expressed in a simple way through the spectral analysis we employed for synchronization and subradiance.

Using the quantities briefly discussed above, Publication **IV** extensively studies how these figures of merit on the capability of the environment to induce collective phenomena vary as a function of the model parameters. In particular, Publication **IV** addresses the question of whether or not synchronization and subradiance can be used as signatures of entanglement generation. The answer is that they are reliable signatures if and only if the qubits are coupled to the environment in a balanced way. That is, if the system-environment coupling constant is the same (or almost the same) for both qubits. Curiously, entanglement generation is always well-captured by a different figure of merit that is analyzed in Publication **IV**, that is, the *collectiveness* of the dynamics introduced in Ref. [115], which is an abstract measure based on the Choi matrix of the open evolution.

Finally, Publication **IV** shows that all these collective effects can emerge for some reasonable model parameters of the circuit in Fig. 3.2. Therefore, quantum synchronization, subradiance and entanglement generation may be observed experimentally using the superconducting circuits that are already available in the laboratories.

3.4 A collision model for *any* Markovian multipartite open quantum system dynamics

In Sec. 2.7 we introduced the concept of "collision models" and we showed how a collision model can simulate a GKLS master equation of a single open system in the limit of infinitesimal timestep. However, the extension of this method to a multipartite open quantum system, that is, the modeling of a quantum

collision model based on elementary collisions between the environment particles and each single subsystem to reproduce global master equations, is not a trivial task[2]. Publication **V** gives a comprehensive answer to this problem, while Publication **VI** builds on these results and presents the implementation of the collision model on a near-term quantum computer. In this section, we will discuss different aspects of this *multipartite collision model.*

3.4.1 Steps of the multipartite collision model

Publication **V** introduces the *multipartite collision model* (MCM), able to reproduce any GKLS master equation of a multipartite open quantum system. This includes both global and local master equations of open quantum systems coupled to common and/or separate baths. Here, we will present the steps of the MCM. Since the MCM can indeed be decomposed into a sequence of steps, and the interactions between subsystems and environment ancillas are elementary (i.e., two-qubit interactions if both the subsystems and the ancillas are qubit), the multipartite collision model can be seen as a quantum algorithm that is easily implementable on a quantum computer.

For simplicity, we will consider here a scenario where the Lindblad operators of the GKLS master equation that we aim to reproduce are linear combinations of operators that are local on each subsystem. Anyway, the MCM works also beyond this scenario. Under this assumption, we can write the GKLS master equation in non-diagonal form as:

$$
\mathcal{L}[\rho_S] = -\frac{i}{\hbar}[\tilde{H}_S, \rho_S] + \sum_{m,\alpha,m',\alpha'} \gamma_{m,\alpha,m',\alpha'} \left(F_{m,\alpha}\rho_S F_{m',\alpha'}^\dagger - \frac{1}{2}\{F_{m',\alpha'}^\dagger F_{m,\alpha}, \rho_S\} \right).
$$
(3.20)

$\tilde{H}_S$ is the effective Hamiltonian of the multipartite open quantum system. The indexes m, m' run over the subsystems (let us say $m, m' = 1, \ldots, M$ if there are M subsystems), while α, α' run over the different local GKS operators of the open dynamics. If the Hilbert space of each subsystem has dimension d, then $\alpha, \alpha' = 1, \ldots, d^2 - 1$, according to the discussion in Sec. 2.3. $F_{m,\alpha}$ is a GKS operator that is local on the subsystem m, while $\gamma_{m,\alpha,m',\alpha'}$ are the coefficients of the master equation[3].

The core idea of the MCM is to use a single ancillary qubit to reproduce each term in the dissipator of Eq. (3.20). This corresponds to one ancilla

---

[2]Some collision models for multipartite systems have been introduced in the past ten years, but they cannot describe a generic GKLS master equation [79, 81, 116].

[3]Note that, for simplicity, in the above equation we are not expressing the fact that, due to the properties of the GKLS master equation that generates a CPTP map, for each term in the master equation with, for example, $F_{m,\alpha}\rho_S F_{m',\alpha'}^\dagger$, there must be a term $F_{m',\alpha'}\rho_S F_{m,\alpha}^\dagger$. We will label both these terms through the same quartet (m, α, m', α').

for each quartet (m, α, m', α'). The way to implement this term by means of collisions is based on the so-called second-order Suzuki-Trotter formula:

$$e^{\frac{\Delta t}{2}A}e^{\Delta t B}e^{\frac{\Delta t}{2}A} = e^{\Delta t(A+B)} + O(\Delta t^3), \qquad (3.21)$$

where $\Delta t \in \mathbb{R}$ and A, B are operators. Then, let us set $A = \lambda_{m,\alpha}F_{m,\alpha} \otimes \sigma_{E,p}^+ + H.c.$ and $B = \lambda_{m',\alpha'}F_{m',\alpha'} \otimes \sigma_{E,p}^+ + H.c.$, where $\sigma_{E,p}^+$ is the operator that creates an excitation in the ancillary qubit associated with $p = (m, \alpha, m', \alpha')$, while $\lambda_{m,\alpha}$ and $\lambda_{m',\alpha'}$ are some constants. Then, $\Delta t(A + B)$ can be used as a single term of the interaction Hamiltonian H_I in Eq. (2.67), which is decomposed into elementary subsystem-ancilla interactions via Eq. (3.21). It can be shown that in this way we are able to reproduce the most general GKLS master equation expressed in Eq. (3.20).

Specifically, the steps of the MCM are the following:

1. For each unordered pair of GKS operators in Eq. (3.20) (i.e., for each quartet $p = (m, \alpha, m', \alpha')$), prepare the collision operators

$$U_p^{(m,\alpha)}(\Delta t) = \exp\left(-\frac{i}{\hbar}g_I \Delta t H_{I,p}^{(m,\alpha)}\right), \qquad (3.22)$$

and analogously for $U_p^{(m',\alpha')}$. In Eq. (3.22), g_I is the magnitude of the collision energy, while $H_{I,p}^{(m,\alpha)} = A$ as defined above (and analogously for m', α' and B). Then, construct the following interaction operator that is expressed according to the second-order Suzuki-Trotter decomposition:

$$U_p(\Delta t) = U_p^{(m,\alpha)}(\Delta t/2)U_p^{(m',\alpha')}(\Delta t)U_p^{(m,\alpha)}(\Delta t/2). \qquad (3.23)$$

2. Compose the interaction operators for all the ancillas as follows:

$$U_I(\Delta t) = \prod_p U_p(\Delta t). \qquad (3.24)$$

The order of the composition can be chosen freely.

3. Add a unitary system evolution with magnitude g_S, according to the discussion in Sec. 2.7:

$$U_{\text{sim}}(\Delta t) = U_S(\Delta t) \circ U_I(\Delta t), \qquad (3.25)$$

where $U_S(\Delta t) = \exp\left(-\frac{i}{\hbar}g_S H_S \Delta t\right)$ and $H_S = \tilde{H}_S/g_S$.

4. Prepare all the ancillas in the ground state[4] $\rho_E(0) = \bigotimes_p |0\rangle_p\langle 0|$.

---

[4]Any diagonal state is actually fine, and in some cases it might be more convenient, for instance, to prepare the ancillas in a thermal state.

5. Build the quantum map of a single timestep of the multipartite collision model as

$$\phi_{\Delta t}[\rho_S] = \mathrm{Tr}_E[U_{\mathrm{sim}}(\Delta t)\rho_S \otimes \rho_E(0)U^{\dagger}_{\mathrm{sim}}(\Delta t)], \qquad (3.26)$$

where the trace is performed over all the ancillas p.

Publication **V** shows that, by properly tuning the constants $\lambda_{m,\alpha}$, we can simulate the Liouvillian $\mathcal{L}$ of any multipartite GKLS master equation through:

$$\exp(\mathcal{L}t) = \lim_{\Delta t \to 0}(\phi_{\Delta t})^n, \quad t = n\Delta t, \qquad (3.27)$$

with the standard assumptions for the magnitudes g_I and g_S introduced in Sec. 2.7. Although to guarantee the complete generality of the MCM we need to assume one ancilla for each pair of GKS operators, Publication **V** discusses some possible shortcuts that highly reduce the number of required ancillas. Moreover, the MCM for a diagonal GKLS equation can also be defined, and further extensions to many-body jump operators and time-dependent Markovian equations are discussed in the original paper.

3.4.2 Theoretical error estimation and simulation efficiency

Publication **V** introduces some measures to quantify the error of the ideal implementation of the MCM when we choose a timestep Δt that is small but not infinitesimal, and derives some upper bounds for this error. While Publication **V** makes use of the one-to-one superoperator norm defined in Eq. (2.19), Publication **VI** extends the error bounds to the diamond norm in Eq. (2.20). Therefore, here we will employ the diamond norm.

The discrepancy between the quantum dynamical semigroup we aim to simulate and the MCM can be captured by the *global error*[5]:

$$\epsilon_g = \|\exp \mathcal{L}t - (\phi_{\Delta t})^n\|_{\diamond}, \quad t = n\Delta t. \qquad (3.28)$$

It can be shown that $\epsilon_g \leq n\epsilon_s$, where the *single-step error* is defined as

$$\epsilon_s = \|\exp \mathcal{L}\Delta t - \phi_{\Delta t}\|_{\diamond}. \qquad (3.29)$$

The single-step error can in turn be bounded through $\epsilon_s \leq \epsilon_t + \epsilon_c$, where the *truncation error* and *collision error* are respectively given by

$$\epsilon_t = \|\exp \mathcal{L}\Delta t - (\mathbb{I}_S + \Delta t\mathcal{L})\|_{\diamond} \text{ and } \epsilon_c = \|\phi_{\Delta t} - (\mathbb{I}_S + \Delta t\mathcal{L})\|_{\diamond}. \qquad (3.30)$$

---

[5]Half of this quantity corresponds to the diamond distance introduced in Eq. (2.21). However, to keep the same notation as in the original papers we do not insert the factor $\frac{1}{2}$.

Publication **V** derives some upper bounds for ϵ_t and ϵ_c, and therefore for the global error of the ideal MCM ϵ_g. We do not show here their expressions because they are quite cumbersome, while we refer the reader to the original paper and to the supplementary material of Publication **V**. We just point out that it can be proven that

$$\epsilon_g \leq O(n\Delta t^2) = O(t^2/n). \tag{3.31}$$

The scaling in Eq. (3.31) can be used to prove that the MCM is efficiently simulable on a quantum computer, under the general assumption of k-local Liouvillian. This means that the Liouvillian can always be decomposed as a sum of terms that act non-trivially on k subsystems only, and the number k is fixed even when the number of subsystems M increases. This assumption is at the basis of quantum simulation [117], and it has been introduced also for the simulation of open quantum systems [118]. The conditions for the efficient simulability of a quantum algorithm require that the number of necessary ancillas and necessary gates scales polynomially as a function of the number of subsystems M, of the time t and of the inverse of the required accuracy $1/\epsilon_g$ [118, 119]. This is what Publication **V** proves for the multipartite collision model.

Publication **VI** extends the study of the theoretical accuracy of the MCM to the case of a noisy collision model. That is, a MCM implemented on a near-term quantum computer with noisy gates and noisy state preparation. For a single timestep of the collision model, we can introduce the more general error

$$\epsilon_{s,n} = \|\exp \mathcal{L}\Delta t - \phi_{\Delta t}^*\|_\diamond, \tag{3.32}$$

where $\phi_{\Delta t}^*$ is the quantum map that describes the actual realization of the MCM on a real quantum computer. Therefore, $\phi_{\Delta t}^*$ is not an ideal algorithm anymore, but contains also some noise that is due to the features of the quantum platform we are using. Using the triangle inequality, this error can be bounded as $\epsilon_{s,n} \leq \epsilon_s + \epsilon_n$, where ϵ_s is the ideal single-step error we introduced in Eq. (3.29), while the *noisy error* is given by

$$\epsilon_n = \|\phi_{\Delta t} - \phi_{\Delta t}^*\|_\diamond. \tag{3.33}$$

The noisy error is therefore describing the discrepancy between the ideal map we aimed to implement on the quantum computer and its actual realization.

Publication **V** gives us an error bound for ϵ_s, while Publication **VI** shows that we can bound ϵ_n using the diamond distances between the ideal and the noisy gates of our quantum computer. More precisely, suppose that we need to employ the sequence of gates $\{\mathcal{U}_j\}_j$ for a single timestep of the MCM. However, we find that their actual implementation can be described by the sequence of

noisy channels $\{\mathcal{E}_j\}_j$. Moreover, suppose that, instead of preparing the state of the ancillas in the desired ground state, we have a noisy state preparation described by the operators $\{\mathcal{G}_i\}_i$ acting on $|0\rangle_i$, where the index i runs over the different ancillas. Then, Publication **VI** proves that the noisy error can be bounded as:

$$\epsilon_n \leq 2 \left(\sum_j d_\diamond(\mathcal{U}_j, \mathcal{E}_j) + \sum_i d_\diamond(\mathbb{I}_E, \mathcal{G}_i) \right), \qquad (3.34)$$

where the diamond distance is given by Eq. (2.21).

3.4.3 Implementation on a near-term quantum computer

In addition to introducing an error bound for the noisy MCM, Publication **VI** presents the experimental results of the simulation of the multipartite collision model on a near-term quantum computer, namely an IBM quantum computer. The experimental results are reported in the original article, while here we will just complement with brief comments about the meaning and validity of these results.

We performed two different kinds of experimental tasks. First, the quantum simulation of the multipartite collision model (up to 5 collisions) to simulate superradiance and subradiance between two qubits, inspired by the study on collective phenomena in Publication **IV**. We point out that experiments showing these collective effects have been already realized in the past, but this is not the main goal of Publication **VI**. Our main goal is to check if we are able to engineer and observe these phenomena via the MCM on the current digital (and not analog) near-term quantum computers. Secondly, we performed the full process tomography [7] of all the CNOT gates we employed in the algorithm, with the aim of better understanding the features of noise on the quantum computer. We have chosen to analyze only the CNOT gates, because it has been shown that the two-qubit gates are by far the noisiest on current near-term computers.

The experimental results of the collision model show a qualitative agreement with the subradiant and superradiant dynamics, at least for the first collisions. That is, we observe a collective evolution that would not be possible in the presence of a local environment acting on each qubit. However, the agreement is only qualitative, and the quantitative precision is low due to the high levels of noise on the platform. After a few collisions, decoherence emerges and the dynamics loses its collective features.

As explained in Sec. 2.2, the full process tomography of the experimental CNOT gates allows us to recover the values of their average gate fidelity in Eq. (2.22) and diamond distance from the ideal gate in Eq. (2.21). Full process

tomography, however, has a drawback: it is subject to the so-called *SPAM errors*, i.e., errors in the state preparation and in the measurements on the circuits for the process tomography [120]. Therefore, we have applied the procedures for error mitigation that are available on the IBM quantum library *qiskit* [121]. Anyway, the results of the process tomography may still contain residual SPAM errors.

Full process tomography allows us to understand some properties of the noise on the quantum computer. First, the diamond distances between experimental and ideal CNOT gates are of the order of 5×10^{-2}–10^{-1}. Since we employ more than 50 CNOT gates to perform five collisions of the algorithm, the cumulative error bound for ϵ_n in Eq. (3.33) is clearly quickly exceeding 1 (note that these distances are exactly the ones employed in Eq. (3.34) for the CNOT gates only). Furthermore, we have compared the experimental value of the average gate infidelity with the gate error provided by IBM, which is estimated through a randomized benchmarking procedure [122]. We have put forward a noise model based on the average gate infidelities of the CNOT gates, and showed that its performance are similar to the one provided by IBM.

To conclude, Publication **VI** shows that signatures of collective phenomena in multipartite open quantum systems can be found also in nowadays near-term digital quantum computers. However, the quantitative accuracy of the quantum simulation is quite low, and the thresholds for the diamond errors of the two-qubit gates are still orders of magnitude away from the experimental diamond distances. Moreover, Publication **VI** performs an extensive noise analysis based on full process tomography, and tries to improve our understanding of the noise we can face on near-term computers and of its relation with the experimental results of the quantum simulation.

Chapter 4

Concluding Remarks

In this thesis we have discussed different aspects of multipartite open quantum systems. We have explained what are the key issues in passing from the description of a generic open quantum system that does not take into account its inner structure to the description of a multipartite system made of multiple subsystems, and how we may develop different methods to solve such issues. Moreover, we have explored the emergence of collective effects in multipartite systems and how to simulate them. In particular, Sec. 3.1 and Publications **I** and **II** focus on the characterization of the master equations for multipartite open quantum systems, while Sec. 3.2 and Publication **III** discusses how we may simulate this type of dynamics on a platform of superconducting qubits. Publication **IV** and Sec. 3.3 are devoted to the study of different collective effects between a pair of qubits in a common bath, which relies on the spectral analysis of the Liouvillian superoperator of the dynamics. Finally, Sec. 3.4 and Publication **V** and **VI** put forward the *multipartite collision model*, which can be seen as a quantum algorithm for the simulation of the most general Markovian dynamics of a multipartite open quantum system, and explore its features both theoretically and experimentally.

The global master equation with partial secular approximation we analyzed in Sec. 3.1 is a useful tool to describe the Markovian dynamics of a generic multipartite open quantum system. Remarkably, it is valid also when the local master equation or the global master equation with full secular approximation fail (i.e., respectively for strong and weak inter-subsystem coupling). Therefore, this master equation may give us a definitive answer to the "local vs global discussion", which animated the communities of open quantum systems and quantum thermodynamics for some years. Moreover, recent results have shown that this master equation can always be slightly modified to obtain a GKLS structure, even if for the sake of numerical simulations we do not always need to use a completely positive master equation.

One missing piece of the discussion on the global master equation with partial secular approximation is its thermodynamic analysis, which will be an interesting outlook for the near future. In particular, Publication **II** proves that this master equation is almost always covariant under the action of a superoperator group generated by the total-number-of-particles operator. This property sets some challenges for the standard resource theories of quantum thermodynamics, which usually assume that the dynamics is covariant under a group generated by the system Hamiltonian. Unifying these two different visions, i.e., making the dynamical constraints coming from thermodynamic assumptions and from the microscopic model of system plus environment agree, promises to be an intriguing challenge for the next few years.

Publication **IV** explores the emergence of subradiance, synchronization and entanglement generation between two detuned qubits in a common bath. This study sheds light on the behavior of these phenomena as a function of the model parameters, and on when and why these effects may appear under the same physical conditions. Extending the results of this work may require to consider more than two subsystems of the multipartite open quantum system. From the theoretical perspective this should be relatively easy, as the theoretical tools we would need to employ (e.g., the master equation and its properties) are still the same. Less trivial is to find a proper figure of merit for these phenomena when the system is not bipartite anymore. On the other hand, Publications **III** and **IV** show that these collective effects can be studied experimentally on a platform of two transmon qubits capacitively coupled to a common resistor, which acts as a thermal bath. Therefore, the most immediate outlook of these works may be their experimental implementation in a circuit QED lab.

The multipartite collision model is a successful tool to reproduce any multipartite GKLS master equation. It can be employed both for quantum thermodynamic studies and for the simulation of the master equation on a quantum computer. Remarkably, Publication **V** also proves that it is efficiently simulable, and to do so it puts forward a procedure to estimate some rigorous error bounds on the global error of the collision model due to a small but finite collision timestep. This procedure can be employed to estimate analogous error bounds for any collision model. Publication **VI** extends these bounds to the presence of experimental errors in the algorithm implementation. Moreover, the experimental results of the multipartite collision model implemented on a near-term quantum computer show signatures of collective effects, although the accuracy of these machines is still quite low due to very noisy two-qubit gates.

Owing to its generality, the multipartite collision model may be immediately applied to simulate fascinating collective phenomena such as the synchronization of extended quantum systems or dissipative time crystals. Fur-

thermore, an interesting outlook of Publication **V** may be the thermodynamic analysis of a single multipartite collision. In what follows we sketch some related questions that are still without an answer: what are the expressions for the production of heat, work and entropy during a single collision? Can we decompose these expressions into some elementary terms associated with a single subsystem only? Is there a difference between these quantities for the multipartite collision model and for a standard unstructured collision model? Can we find a qualitative difference in these expressions when we pass from the description of a local master equation to a highly global one? Addressing these issues would provide a remarkable step forward for the thermodynamics of multipartite quantum systems. Moreover, Publication **VI** paves the way for the experimental study of the thermodynamics of the multipartite collision model on a near-term quantum computer.

In conclusion, the field of multipartite open quantum systems is getting more and more important for contemporary quantum mechanics, due to the increasing number of theoretical and experimental studies focused on extended quantum systems, which are crucial, for instance, for the future of quantum computation and simulation. This thesis presents some relevant results on the study and characterization of multipartite open quantum systems. We hope the readers will appreciate these contributions in this era of excitement and discoveries on quantum technologies and fundamental quantum physics, when a more structured and accurate characterization of the quantum systems we manipulate is deemed necessary.

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